Crystallographic details of CMS 56

Table 1. Crystal data and structure refinement for CMS.

Identification code	CMS
Empirical formula	C23 H36 Cu N2 O4
Formula weight	468.08
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 11.0626(2) A alpha = 90 deg. b = 12.0807(3) A beta = 90 deg. c = 16.4661(4) A gamma = 90 deg.
Volume	2200.59(9) A^3
Z, Calculated density	4, 1.413 Mg/m^3
Absorption coefficient	1.024 mm^-1
F(000)	996
Crystal size	0.30 x 0.20 x 0.04 mm
Theta range for data collection	2.22 to 27.52 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -21<=l<=21
Reflections collected / unique	10090 / 5070 [R(int) = 0.0463]
Completeness to theta = 27.52	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5070 / 0 / 288
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0684
R indices (all data)	R1 = 0.0625, wR2 = 0.0747
Absolute structure parameter	0.005(11)
Largest diff. peak and hole	0.349 and -0.320 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for CMS. U(eq) is defined as one third of the trace of the Orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	6941(1)	9763(1)	8434(1)	17(1)
O(1)	7951(2)	8796(2)	9112(1)	23(1)
O(2)	6412(2)	7686(2)	8819(1)	29(1)
O(3)	6127(2)	10290(2)	9429(1)	23(1)
O(4)	7235(2)	11711(2)	9029(1)	32(1)
N(1)	8008(2)	9551(2)	7426(1)	18(1)
N(2)	5531(2)	10187(2)	7660(1)	17(1)
C(1)	9267(2)	9239(2)	7657(2)	21(1)
C(2)	9884(2)	10173(2)	8120(2)	24(1)
C(3)	9956(3)	11211(2)	7601(2)	25(1)
C(4)	8689(3)	11512(2)	7293(2)	24(1)
C(5)	8085(3)	10543(2)	6871(2)	20(1)
C(6)	6851(2)	10810(2)	6506(2)	21(1)
C(7)	6423(2)	9829(2)	5998(2)	24(1)
C(8)	6252(2)	8866(2)	6591(2)	23(1)
C(9)	7473(2)	8604(2)	6982(2)	22(1)
C(10)	5868(2)	11118(2)	7113(2)	20(1)
C(11)	5240(2)	9122(2)	7209(2)	19(1)
C(12)	4002(2)	9122(2)	6793(2)	23(1)
C(13)	2987(3)	9435(2)	7362(2)	27(1)
C(14)	3251(2)	10566(2)	7717(2)	25(1)
C(15)	4457(2)	10515(2)	8169(2)	20(1)
C(16)	7387(3)	7874(2)	9171(2)	21(1)
C(17)	7967(3)	6994(2)	9684(2)	28(1)
C(18)	9227(3)	7042(3)	9826(3)	41(1)
C(19)	7229(3)	6136(3)	9998(2)	45(1)
C(20)	6451(3)	11306(3)	9476(2)	23(1)
C(21)	5810(3)	12030(2)	10079(2)	28(1)
C(22)	6371(4)	13102(3)	10265(2)	53(1)
C(23)	4740(4)	11687(4)	10382(2)	49(1)

Table 3. Bond lengths [A] and angles [deg] for CMS.

Cu(1)-O(1)	1.9654(18)
Cu(1)-O(3)	1.9743(17)
Cu(1)-N(1)	2.054(2)
Cu(1)-N(2)	2.078(2)
O(1)-C(16)	1.280(3)
O(2)-C(16)	1.245(3)
O(3)-C(20)	1.281(3)
O(4)-C(20)	1.239(3)
N(1)-C(9)	1.480(3)
N(1)-C(1)	1.493(3)

N(1)-C(5)	1.509(3)
N(2)-C(10)	1.488(3)
N(2)-C(15)	1.507(3)
N(2)-C(11)	1.520(3)
C(1)-C(2)	1.523(4)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.520(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.534(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.517(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.526(4)
C(5)-H(5)	1.0000
C(6)-C(10)	1.524(4)
C(6)-C(7)	1.526(4)
C(6)-H(6)	1.0000
C(7)-C(8)	1.530(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.530(4)
C(8)-C(11)	1.543(4)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.531(4)
C(11)-H(11)	1.0000
C(12)-C(13)	1.512(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.514(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.528(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.502(4)
C(17)-C(18)	1.414(5)
C(17)-C(19)	1.417(4)
C(18)-H(18B)	0.81(3)
C(18)-H(18A)	0.81(3)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.501(4)
C(21)-C(23)	1.350(5)
C(21)-C(22)	1.468(4)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800

C(22)-H(22C)	0.9800
C(23)-H(23A)	0.92(3)
C(23)-H(23B)	0.86(4)
O(1)-Cu(1)-O(3)	88.84(8)
O(1)-Cu(1)-N(1)	93.31(8)
O(3)-Cu(1)-N(1)	166.73(8)
O(1)-Cu(1)-N(2)	157.18(8)
O(3)-Cu(1)-N(2)	95.05(8)
N(1)-Cu(1)-N(2)	88.03(8)
C(16)-O(1)-Cu(1)	106.40(17)
C(20)-O(3)-Cu(1)	103.38(17)
C(9)-N(1)-C(1)	107.68(19)
C(9)-N(1)-C(5)	109.74(19)
C(1)-N(1)-C(5)	107.6(2)
C(9)-N(1)-Cu(1)	105.44(16)
C(1)-N(1)-Cu(1)	111.19(15)
C(5)-N(1)-Cu(1)	114.99(15)
C(10)-N(2)-C(15)	109.6(2)
C(10)-N(2)-C(11)	113.41(19)
C(15)-N(2)-C(11)	109.10(19)
C(10)-N(2)-Cu(1)	111.67(16)
C(15)-N(2)-Cu(1)	108.36(14)
C(11)-N(2)-Cu(1)	104.51(15)
N(1)-C(1)-C(2)	111.1(2)
N(1)-C(1)-H(1A)	109.4
C(2)-C(1)-H(1A)	109.4
N(1)-C(1)-H(1B)	109.4
C(2)-C(1)-H(1B)	109.4
H(1A)-C(1)-H(1B)	108.0
C(3)-C(2)-C(1)	110.7(2)
C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
C(2)-C(3)-C(4)	109.5(2)
C(2)-C(3)-H(3A)	109.8
C(4)-C(3)-H(3A)	109.8
C(2)-C(3)-H(3B)	109.8
C(4)-C(3)-H(3B)	109.8
H(3A)-C(3)-H(3B)	108.2
C(5)-C(4)-C(3)	111.7(2)
C(5)-C(4)-H(4A)	109.3
C(3)-C(4)-H(4A)	109.3
C(5)-C(4)-H(4B)	109.3
C(3)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	107.9
N(1)-C(5)-C(4)	111.1(2)
N(1)-C(5)-C(6)	110.8(2)
C(4)-C(5)-C(6)	114.3(2)
N(1)-C(5)-H(5)	106.7
C(4)-C(5)-H(5)	106.7
C(6)-C(5)-H(5)	106.7
C(10)-C(6)-C(7)	109.2(2)
C(10)-C(6)-C(5)	115.5(2)
C(7)-C(6)-C(5)	109.2(2)

C(10)-C(6)-H(6)	107.5
C(7)-C(6)-H(6)	107.5
C(5)-C(6)-H(6)	107.5
C(6)-C(7)-C(8)	106.2(2)
C(6)-C(7)-H(7A)	110.5
C(8)-C(7)-H(7A)	110.5
C(6)-C(7)-H(7B)	110.5
C(8)-C(7)-H(7B)	110.5
H(7A)-C(7)-H(7B)	108.7
C(9)-C(8)-C(7)	108.5(2)
C(9)-C(8)-C(11)	113.9(2)
C(7)-C(8)-C(11)	111.0(2)
C(9)-C(8)-H(8)	107.8
C(7)-C(8)-H(8)	107.8
C(11)-C(8)-H(8)	107.8
N(1)-C(9)-C(8)	113.6(2)
N(1)-C(9)-H(9A)	108.8
C(8)-C(9)-H(9A)	108.8
N(1)-C(9)-H(9B)	108.8
C(8)-C(9)-H(9B)	108.8
H(9A)-C(9)-H(9B)	107.7
N(2)-C(10)-C(6)	113.0(2)
N(2)-C(10)-H(10A)	109.0
C(6)-C(10)-H(10A)	109.0
N(2)-C(10)-H(10B)	109.0
C(6)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
N(2)-C(11)-C(12)	114.1(2)
N(2)-C(11)-C(8)	109.7(2)
C(12)-C(11)-C(8)	110.7(2)
N(2)-C(11)-H(11)	107.3
C(12)-C(11)-H(11)	107.3
C(8)-C(11)-H(11)	107.3
C(13)-C(12)-C(11)	112.8(2)
C(13)-C(12)-H(12A)	109.0
C(11)-C(12)-H(12A)	109.0
C(13)-C(12)-H(12B)	109.0
C(11)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
C(12)-C(13)-C(14)	108.8(2)
C(12)-C(13)-H(13A)	109.9
C(14)-C(13)-H(13A)	109.9
C(12)-C(13)-H(13B)	109.9
C(14)-C(13)-H(13B)	109.9
H(13A)-C(13)-H(13B)	108.3
C(13)-C(14)-C(15)	108.7(2)
C(13)-C(14)-H(14A)	109.9
C(15)-C(14)-H(14A)	109.9
C(13)-C(14)-H(14B)	109.9
C(15)-C(14)-H(14B)	109.9
H(14A)-C(14)-H(14B)	108.3
N(2)-C(15)-C(14)	115.4(2)
N(2)-C(15)-H(15A)	108.4
C(14)-C(15)-H(15A)	108.4
N(2)-C(15)-H(15B)	108.4
C(14)-C(15)-H(15B)	108.4
H(15A)-C(15)-H(15B)	107.5

O(2)-C(16)-O(1)	123.1(3)
O(2)-C(16)-C(17)	120.2(3)
O(1)-C(16)-C(17)	116.7(3)
C(18)-C(17)-C(19)	122.5(3)
C(18)-C(17)-C(16)	119.0(3)
C(19)-C(17)-C(16)	118.5(3)
C(17)-C(18)-H(18B)	114(2)
C(17)-C(18)-H(18A)	115(2)
H(18B)-C(18)-H(18A)	128(3)
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(4)-C(20)-O(3)	122.6(3)
O(4)-C(20)-C(21)	119.6(3)
O(3)-C(20)-C(21)	117.8(3)
C(23)-C(21)-C(22)	124.4(3)
C(23)-C(21)-C(20)	118.6(3)
C(22)-C(21)-C(20)	116.9(3)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	126(2)
C(21)-C(23)-H(23B)	113(2)
H(23A)-C(23)-H(23B)	122(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for CMS. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	18(1)	16(1)	18(1)	0(1)	0(1)	0(1)
O(1)	22(1)	23(1)	24(1)	6(1)	-3(1)	2(1)
O(2)	28(1)	32(1)	27(1)	3(1)	-3(1)	-2(1)
O(3)	24(1)	23(1)	21(1)	-3(1)	-1(1)	2(1)
O(4)	42(1)	28(1)	26(1)	-1(1)	2(1)	0(1)
N(1)	16(1)	16(1)	21(1)	1(1)	1(1)	-1(1)
N(2)	16(1)	16(1)	20(1)	-1(1)	1(1)	1(1)
C(1)	19(2)	20(2)	23(2)	1(1)	3(1)	6(1)
C(2)	16(1)	25(1)	30(1)	2(1)	2(1)	-1(1)
C(3)	23(2)	22(2)	32(2)	1(1)	2(1)	-3(1)
C(4)	24(2)	17(2)	30(2)	5(1)	3(1)	-1(1)
C(5)	19(1)	21(1)	21(1)	3(1)	5(1)	-2(1)

C(6)	21(1)	21(1)	21(1)	7(1)	-2(2)	2(1)
C(7)	22(1)	32(2)	17(1)	1(1)	-2(1)	2(1)
C(8)	25(2)	23(2)	21(1)	-7(2)	-1(1)	-1(1)
C(9)	23(2)	19(2)	23(2)	-8(1)	1(1)	2(1)
C(10)	20(2)	16(1)	24(2)	2(1)	1(1)	0(1)
C(11)	22(2)	14(2)	20(1)	-3(1)	-3(1)	-1(1)
C(12)	22(2)	22(2)	24(2)	-1(1)	-4(1)	-2(1)
C(13)	19(2)	30(2)	32(2)	3(1)	-3(1)	-3(1)
C(14)	18(2)	29(2)	27(2)	1(1)	3(1)	4(1)
C(15)	17(1)	22(2)	22(1)	-1(1)	4(1)	-1(1)
C(16)	24(2)	24(2)	16(2)	-1(1)	2(1)	6(1)
C(17)	41(2)	23(2)	19(2)	-2(1)	-1(2)	6(2)
C(18)	30(2)	42(2)	50(2)	24(2)	-8(2)	5(2)
C(19)	60(2)	31(2)	43(2)	10(2)	-14(2)	-6(2)
C(20)	26(2)	26(2)	17(2)	-1(1)	-7(1)	8(1)
C(21)	39(2)	29(2)	17(2)	1(1)	-5(1)	10(2)
C(22)	109(3)	26(2)	24(2)	-3(2)	1(2)	18(2)
C(23)	46(3)	64(3)	37(2)	-26(2)	-6(2)	24(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for CMS.

	x	y	z	U(eq)
H(1A)	9737	9067	7161	25
H(1B)	9248	8566	8000	25
H(2A)	9425	10334	8622	28
H(2B)	10710	9940	8278	28
H(3A)	10502	11082	7134	30
H(3B)	10288	11830	7926	30
H(4A)	8183	11751	7757	28
H(4B)	8750	12141	6910	28
H(5)	8623	10328	6409	24
H(6)	6958	11452	6130	25
H(7A)	7032	9638	5581	29
H(7B)	5651	10006	5723	29
H(8)	5998	8204	6270	28
H(9A)	7370	7978	7364	26
H(9B)	8044	8365	6553	26
H(10A)	6153	11748	7447	24
H(10B)	5141	11364	6813	24
H(11)	5237	8510	7617	23
H(12A)	4018	9649	6333	27
H(12B)	3842	8375	6569	27
H(13A)	2920	8881	7803	33
H(13B)	2211	9453	7063	33
H(14A)	2598	10782	8096	30
H(14B)	3293	11124	7278	30
H(15A)	4619	11251	8409	24
H(15B)	4379	9981	8622	24
H(19A)	6979	5645	9556	67

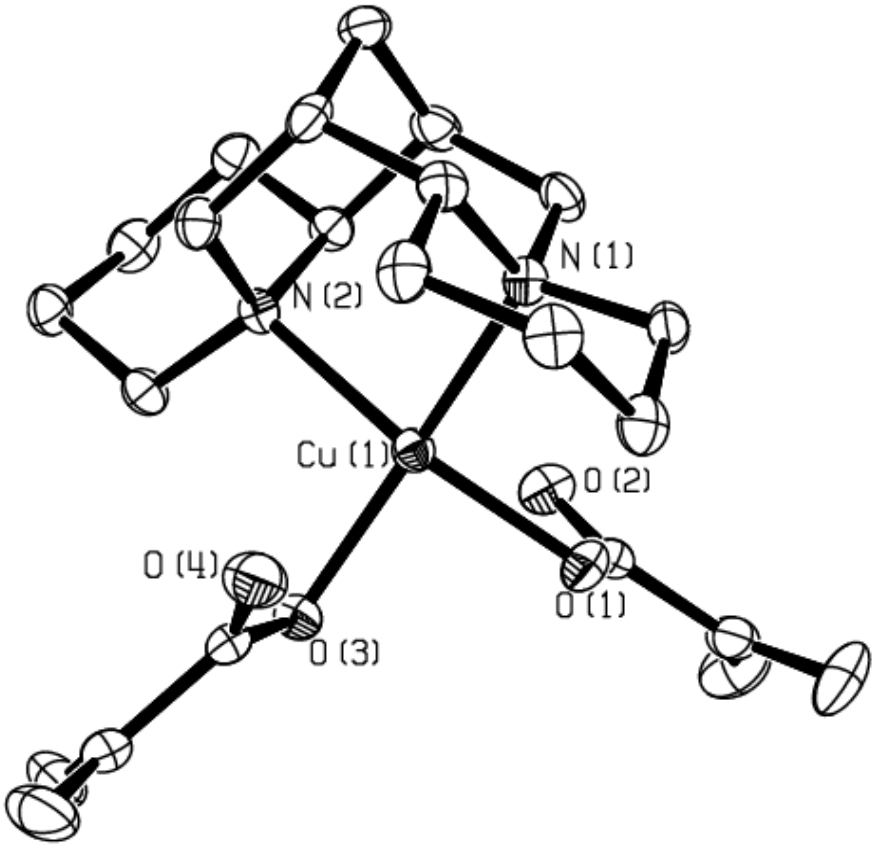
H(19B)	6512	6459	10255	67
H(19C)	7686	5712	10402	67
H(22A)	5809	13552	10585	79
H(22B)	6565	13487	9758	79
H(22C)	7114	12982	10577	79
H(23A)	4380(30)	11010(30)	10275(19)	39(11)
H(23B)	4430(30)	12150(30)	10720(20)	62(12)
H(18B)	9480(30)	6530(20)	10100(20)	36(10)
H(18A)	9600(30)	7430(30)	9510(20)	40(11)

Table 6. Torsion angles [deg] for CMS.

O(3)-Cu(1)-O(1)-C(16)	90.07(17)
N(1)-Cu(1)-O(1)-C(16)	-103.04(17)
N(2)-Cu(1)-O(1)-C(16)	-10.2(3)
O(1)-Cu(1)-O(3)-C(20)	113.08(17)
N(1)-Cu(1)-O(3)-C(20)	13.5(4)
N(2)-Cu(1)-O(3)-C(20)	-89.45(17)
O(1)-Cu(1)-N(1)-C(9)	91.92(16)
O(3)-Cu(1)-N(1)-C(9)	-169.1(3)
N(2)-Cu(1)-N(1)-C(9)	-65.27(16)
O(1)-Cu(1)-N(1)-C(1)	-24.49(16)
O(3)-Cu(1)-N(1)-C(1)	74.5(4)
N(2)-Cu(1)-N(1)-C(1)	178.31(16)
O(1)-Cu(1)-N(1)-C(5)	-147.06(18)
O(3)-Cu(1)-N(1)-C(5)	-48.0(5)
N(2)-Cu(1)-N(1)-C(5)	55.75(18)
O(1)-Cu(1)-N(2)-C(10)	-149.4(2)
O(3)-Cu(1)-N(2)-C(10)	111.54(16)
N(1)-Cu(1)-N(2)-C(10)	-55.53(17)
O(1)-Cu(1)-N(2)-C(15)	89.8(3)
O(3)-Cu(1)-N(2)-C(15)	-9.24(17)
N(1)-Cu(1)-N(2)-C(15)	-176.30(16)
O(1)-Cu(1)-N(2)-C(11)	-26.4(3)
O(3)-Cu(1)-N(2)-C(11)	-125.47(15)
N(1)-Cu(1)-N(2)-C(11)	67.46(15)
C(9)-N(1)-C(1)-C(2)	-179.9(2)
C(5)-N(1)-C(1)-C(2)	61.9(2)
Cu(1)-N(1)-C(1)-C(2)	-64.9(2)
N(1)-C(1)-C(2)-C(3)	-60.5(3)
C(1)-C(2)-C(3)-C(4)	54.1(3)
C(2)-C(3)-C(4)-C(5)	-53.1(3)
C(9)-N(1)-C(5)-C(4)	-177.1(2)
C(1)-N(1)-C(5)-C(4)	-60.2(3)
Cu(1)-N(1)-C(5)-C(4)	64.3(3)
C(9)-N(1)-C(5)-C(6)	54.7(3)
C(1)-N(1)-C(5)-C(6)	171.6(2)
Cu(1)-N(1)-C(5)-C(6)	-63.9(2)
C(3)-C(4)-C(5)-N(1)	57.1(3)
C(3)-C(4)-C(5)-C(6)	-176.5(2)
N(1)-C(5)-C(6)-C(10)	62.0(3)

C(4)-C(5)-C(6)-C(10)	-64.6(3)
N(1)-C(5)-C(6)-C(7)	-61.6(3)
C(4)-C(5)-C(6)-C(7)	171.9(2)
C(10)-C(6)-C(7)-C(8)	-62.9(3)
C(5)-C(6)-C(7)-C(8)	64.3(3)
C(6)-C(7)-C(8)-C(9)	-61.7(3)
C(6)-C(7)-C(8)-C(11)	64.1(3)
C(1)-N(1)-C(9)-C(8)	-171.1(2)
C(5)-N(1)-C(9)-C(8)	-54.2(3)
Cu(1)-N(1)-C(9)-C(8)	70.2(2)
C(7)-C(8)-C(9)-N(1)	58.9(3)
C(11)-C(8)-C(9)-N(1)	-65.1(3)
C(15)-N(2)-C(10)-C(6)	-173.1(2)
C(11)-N(2)-C(10)-C(6)	-50.9(3)
Cu(1)-N(2)-C(10)-C(6)	66.8(2)
C(7)-C(6)-C(10)-N(2)	57.9(3)
C(5)-C(6)-C(10)-N(2)	-65.7(3)
C(10)-N(2)-C(11)-C(12)	-75.6(3)
C(15)-N(2)-C(11)-C(12)	46.8(3)
Cu(1)-N(2)-C(11)-C(12)	162.55(18)
C(10)-N(2)-C(11)-C(8)	49.3(3)
C(15)-N(2)-C(11)-C(8)	171.8(2)
Cu(1)-N(2)-C(11)-C(8)	-72.5(2)
C(9)-C(8)-C(11)-N(2)	65.7(3)
C(7)-C(8)-C(11)-N(2)	-57.0(3)
C(9)-C(8)-C(11)-C(12)	-167.5(2)
C(7)-C(8)-C(11)-C(12)	69.8(3)
N(2)-C(11)-C(12)-C(13)	-52.2(3)
C(8)-C(11)-C(12)-C(13)	-176.6(2)
C(11)-C(12)-C(13)-C(14)	57.3(3)
C(12)-C(13)-C(14)-C(15)	-59.1(3)
C(10)-N(2)-C(15)-C(14)	73.0(3)
C(11)-N(2)-C(15)-C(14)	-51.7(3)
Cu(1)-N(2)-C(15)-C(14)	-164.95(18)
C(13)-C(14)-C(15)-N(2)	59.3(3)
Cu(1)-O(1)-C(16)-O(2)	2.5(3)
Cu(1)-O(1)-C(16)-C(17)	-178.43(18)
O(2)-C(16)-C(17)-C(18)	156.7(3)
O(1)-C(16)-C(17)-C(18)	-22.4(4)
O(2)-C(16)-C(17)-C(19)	-22.5(4)
O(1)-C(16)-C(17)-C(19)	158.4(3)
Cu(1)-O(3)-C(20)-O(4)	-8.9(3)
Cu(1)-O(3)-C(20)-C(21)	168.6(2)
O(4)-C(20)-C(21)-C(23)	160.2(3)
O(3)-C(20)-C(21)-C(23)	-17.4(4)
O(4)-C(20)-C(21)-C(22)	-16.6(4)
O(3)-C(20)-C(21)-C(22)	165.8(3)

Symmetry transformations used to generate equivalent atoms:



Crystal structure of CMS

Crystallographic details of CMN 57

Table 1. Crystal data and structure refinement for CMN.

Identification code	CMN
Empirical formula	C18 H24 Cu N2 O4
Formula weight	395.93
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P1
Unit cell dimensions	a = 9.5553(2) A alpha = 104.235(1) deg. b = 9.6147(2) A beta = 107.076(1) deg. c = 11.1816(3) A gamma = 96.800(1) deg.
Volume	931.47(4) A^3
Z, Calculated density	2, 1.412 Mg/m^3
Absorption coefficient	1.196 mm^-1
F(000)	414
Crystal size	0.20 x 0.20 x 0.18 mm
Theta range for data collection	1.99 to 27.02 deg.
Limiting indices	-12<=h<=12, -12<=k<=12, -14<=l<=14
Reflections collected / unique	8130 / 8130 [R(int) = 0.0000]
Completeness to theta = 27.02	99.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8130 / 3 / 458
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0687
R indices (all data)	R1 = 0.0521, wR2 = 0.0746
Absolute structure parameter	0.024(11)
Largest diff. peak and hole	0.321 and -0.284 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for CMN. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	3755(1)	8623(1)	8629(1)	27(1)
Cu(2)	2934(1)	9244(1)	6396(1)	26(1)
O(1)	5749(4)	9573(4)	8768(3)	34(1)
O(2)	5078(4)	10015(4)	6816(4)	35(1)
O(3)	3974(4)	6804(4)	7446(3)	33(1)
O(4)	3219(4)	7301(4)	5527(3)	33(1)
O(5)	1635(4)	7773(4)	8223(4)	35(1)
O(6)	924(3)	8343(4)	6338(3)	32(1)
O(7)	3356(4)	10551(4)	9432(3)	32(1)
O(8)	2761(4)	11105(4)	7535(3)	33(1)
N(1)	4574(4)	7852(4)	10324(4)	26(1)
N(2)	7729(3)	5088(3)	10372(3)	34(1)
N(3)	2019(4)	10046(4)	4738(4)	26(1)
N(4)	-1445(3)	13141(3)	3675(3)	33(1)
C(1)	3873(5)	7891(5)	11206(4)	26(1)
C(2)	4354(5)	7339(5)	12240(4)	33(1)
C(3)	5608(5)	6717(5)	12377(4)	32(1)
C(4)	6341(4)	6648(4)	11478(4)	28(1)
C(5)	5784(5)	7233(5)	10446(5)	30(1)
C(6)	7705(4)	5979(4)	11609(4)	34(1)
C(7)	9199(6)	7114(6)	12137(7)	56(2)
C(8)	10246(5)	6258(5)	11602(5)	58(1)
C(9)	9252(4)	4784(4)	10686(4)	46(1)
C(10)	6591(5)	3769(5)	9812(4)	45(1)
C(11)	2549(5)	10109(5)	3777(5)	32(1)
C(12)	1882(5)	10700(5)	2785(4)	33(1)
C(13)	631(5)	11265(5)	2820(5)	34(1)
C(14)	54(5)	11217(5)	3809(4)	29(1)
C(15)	807(5)	10594(5)	4732(5)	28(1)
C(16)	-1355(4)	11733(4)	3904(4)	29(1)
C(17)	-2788(5)	10757(6)	2872(6)	51(2)
C(18)	-3927(5)	11755(5)	2805(5)	55(1)
C(19)	-2972(4)	13276(4)	3604(4)	39(1)
C(20)	-309(5)	14339(5)	4679(5)	53(1)
C(21)	6035(5)	10026(6)	7875(6)	32(1)
C(22)	7657(5)	10627(6)	8090(5)	37(1)
C(23)	8718(6)	10510(7)	9171(6)	49(2)
C(24)	7949(6)	11284(6)	7149(6)	49(2)
C(25)	3690(5)	6500(5)	6223(5)	28(1)
C(26)	3960(5)	5045(5)	5543(5)	27(1)
C(27)	4478(6)	4100(6)	6306(5)	39(1)
C(28)	3671(6)	4689(6)	4193(5)	34(1)
C(29)	666(5)	7830(5)	7199(5)	27(1)
C(30)	-934(5)	7254(6)	7014(5)	35(1)
C(31)	-1248(7)	6577(7)	7976(6)	59(2)
C(32)	-2050(6)	7397(6)	5990(6)	44(1)
C(33)	2935(5)	11386(5)	8732(5)	25(1)
C(34)	2621(5)	12841(5)	9374(5)	28(1)
C(35)	2810(6)	13199(6)	10727(5)	35(1)
C(36)	2163(6)	13772(6)	8611(5)	36(1)

Table 3. Bond lengths [A] and angles [deg] for CMN.

Cu(1)-O(1)	1.958(3)
Cu(1)-O(5)	1.965(4)
Cu(1)-O(7)	1.985(3)
Cu(1)-O(3)	1.991(3)
Cu(1)-N(1)	2.171(4)
Cu(1)-Cu(2)	2.6273(4)
Cu(2)-O(2)	1.967(4)
Cu(2)-O(4)	1.972(3)
Cu(2)-O(8)	1.981(3)
Cu(2)-O(6)	1.988(3)
Cu(2)-N(3)	2.169(4)
O(1)-C(21)	1.267(6)
O(2)-C(21)	1.263(6)
O(3)-C(25)	1.262(6)
O(4)-C(25)	1.255(6)
O(5)-C(29)	1.262(6)
O(6)-C(29)	1.255(6)
O(7)-C(33)	1.273(5)
O(8)-C(33)	1.253(6)
N(1)-C(1)	1.341(6)
N(1)-C(5)	1.349(6)
N(2)-C(10)	1.437(5)
N(2)-C(6)	1.446(4)
N(2)-C(9)	1.476(4)
N(3)-C(11)	1.326(6)
N(3)-C(15)	1.326(6)
N(4)-C(16)	1.446(4)
N(4)-C(20)	1.455(5)
N(4)-C(19)	1.461(4)
C(1)-C(2)	1.370(6)
C(1)-H(1)	0.9500
C(2)-C(3)	1.387(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.378(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.400(6)
C(4)-C(6)	1.506(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.548(6)
C(6)-H(6)	1.0000
C(7)-C(8)	1.530(7)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.534(6)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.393(6)
C(11)-H(11)	0.9500

C(12)-C(13)	1.378(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.380(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.383(6)
C(14)-C(16)	1.512(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.524(6)
C(16)-H(16)	1.0000
C(17)-C(18)	1.532(6)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.527(6)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.515(7)
C(22)-C(23)	1.369(8)
C(22)-C(24)	1.428(7)
C(23)-H(23A)	0.9500
C(23)-H(23B)	0.9500
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.510(6)
C(26)-C(28)	1.397(7)
C(26)-C(27)	1.427(7)
C(27)-H(27A)	0.9500
C(27)-H(27B)	0.9500
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.498(7)
C(30)-C(32)	1.365(8)
C(30)-C(31)	1.468(8)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9500
C(32)-H(32B)	0.9500
C(33)-C(34)	1.515(6)
C(34)-C(36)	1.404(7)
C(34)-C(35)	1.417(7)
C(35)-H(35A)	0.9500
C(35)-H(35B)	0.9500
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800

O(1)-Cu(1)-O(5)	170.38(15)
O(1)-Cu(1)-O(7)	90.39(15)
O(5)-Cu(1)-O(7)	88.13(15)
O(1)-Cu(1)-O(3)	89.09(15)

O(5)-Cu(1)-O(3)	90.21(15)
O(7)-Cu(1)-O(3)	166.95(13)
O(1)-Cu(1)-N(1)	94.06(14)
O(5)-Cu(1)-N(1)	95.55(14)
O(7)-Cu(1)-N(1)	101.63(14)
O(3)-Cu(1)-N(1)	91.42(13)
O(1)-Cu(1)-Cu(2)	83.49(10)
O(5)-Cu(1)-Cu(2)	86.93(10)
O(7)-Cu(1)-Cu(2)	86.74(9)
O(3)-Cu(1)-Cu(2)	80.24(9)
N(1)-Cu(1)-Cu(2)	171.32(10)
O(2)-Cu(2)-O(4)	88.75(15)
O(2)-Cu(2)-O(8)	90.23(15)
O(4)-Cu(2)-O(8)	170.61(14)
O(2)-Cu(2)-O(6)	167.17(14)
O(4)-Cu(2)-O(6)	90.25(14)
O(8)-Cu(2)-O(6)	88.67(14)
O(2)-Cu(2)-N(3)	99.68(15)
O(4)-Cu(2)-N(3)	101.66(14)
O(8)-Cu(2)-N(3)	87.71(14)
O(6)-Cu(2)-N(3)	93.05(14)
O(2)-Cu(2)-Cu(1)	85.36(10)
O(4)-Cu(2)-Cu(1)	88.60(10)
O(8)-Cu(2)-Cu(1)	82.01(9)
O(6)-Cu(2)-Cu(1)	81.83(10)
N(3)-Cu(2)-Cu(1)	168.60(10)
C(21)-O(1)-Cu(1)	124.0(3)
C(21)-O(2)-Cu(2)	121.6(3)
C(25)-O(3)-Cu(1)	126.9(3)
C(25)-O(4)-Cu(2)	118.2(3)
C(29)-O(5)-Cu(1)	120.2(3)
C(29)-O(6)-Cu(2)	125.2(3)
C(33)-O(7)-Cu(1)	119.9(3)
C(33)-O(8)-Cu(2)	126.0(3)
C(1)-N(1)-C(5)	119.1(4)
C(1)-N(1)-Cu(1)	122.5(3)
C(5)-N(1)-Cu(1)	118.3(3)
C(10)-N(2)-C(6)	113.2(3)
C(10)-N(2)-C(9)	112.4(3)
C(6)-N(2)-C(9)	103.8(3)
C(11)-N(3)-C(15)	116.9(4)
C(11)-N(3)-Cu(2)	128.4(3)
C(15)-N(3)-Cu(2)	114.7(3)
C(16)-N(4)-C(20)	113.1(3)
C(16)-N(4)-C(19)	103.1(2)
C(20)-N(4)-C(19)	113.5(3)
N(1)-C(1)-C(2)	122.3(4)
N(1)-C(1)-H(1)	118.9
C(2)-C(1)-H(1)	118.9
C(1)-C(2)-C(3)	118.8(4)
C(1)-C(2)-H(2)	120.6
C(3)-C(2)-H(2)	120.6
C(4)-C(3)-C(2)	120.2(4)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	117.8(4)
C(3)-C(4)-C(6)	121.0(4)

C(5)-C(4)-C(6)	121.2(4)
N(1)-C(5)-C(4)	121.9(4)
N(1)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
N(2)-C(6)-C(4)	113.0(3)
N(2)-C(6)-C(7)	103.0(4)
C(4)-C(6)-C(7)	114.1(3)
N(2)-C(6)-H(6)	108.8
C(4)-C(6)-H(6)	108.8
C(7)-C(6)-H(6)	108.8
C(8)-C(7)-C(6)	103.3(4)
C(8)-C(7)-H(7A)	111.1
C(6)-C(7)-H(7A)	111.1
C(8)-C(7)-H(7B)	111.1
C(6)-C(7)-H(7B)	111.1
H(7A)-C(7)-H(7B)	109.1
C(7)-C(8)-C(9)	105.4(4)
C(7)-C(8)-H(8A)	110.7
C(9)-C(8)-H(8A)	110.7
C(7)-C(8)-H(8B)	110.7
C(9)-C(8)-H(8B)	110.7
H(8A)-C(8)-H(8B)	108.8
N(2)-C(9)-C(8)	103.6(3)
N(2)-C(9)-H(9A)	111.0
C(8)-C(9)-H(9A)	111.0
N(2)-C(9)-H(9B)	111.0
C(8)-C(9)-H(9B)	111.0
H(9A)-C(9)-H(9B)	109.0
N(2)-C(10)-H(10A)	109.5
N(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
N(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(12)	122.9(4)
N(3)-C(11)-H(11)	118.5
C(12)-C(11)-H(11)	118.5
C(13)-C(12)-C(11)	118.3(4)
C(13)-C(12)-H(12)	120.9
C(11)-C(12)-H(12)	120.9
C(12)-C(13)-C(14)	120.1(4)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(13)-C(14)-C(15)	116.2(4)
C(13)-C(14)-C(16)	124.5(4)
C(15)-C(14)-C(16)	119.2(4)
N(3)-C(15)-C(14)	125.5(4)
N(3)-C(15)-H(15)	117.2
C(14)-C(15)-H(15)	117.2
N(4)-C(16)-C(14)	113.7(3)
N(4)-C(16)-C(17)	101.9(3)
C(14)-C(16)-C(17)	114.0(4)
N(4)-C(16)-H(16)	109.0
C(14)-C(16)-H(16)	109.0
C(17)-C(16)-H(16)	109.0
C(16)-C(17)-C(18)	104.0(4)
C(16)-C(17)-H(17A)	111.0

C(18)-C(17)-H(17A)	111.0
C(16)-C(17)-H(17B)	111.0
C(18)-C(17)-H(17B)	111.0
H(17A)-C(17)-H(17B)	109.0
C(19)-C(18)-C(17)	103.6(3)
C(19)-C(18)-H(18A)	111.0
C(17)-C(18)-H(18A)	111.0
C(19)-C(18)-H(18B)	111.0
C(17)-C(18)-H(18B)	111.0
H(18A)-C(18)-H(18B)	109.0
N(4)-C(19)-C(18)	104.8(3)
N(4)-C(19)-H(19A)	110.8
C(18)-C(19)-H(19A)	110.8
N(4)-C(19)-H(19B)	110.8
C(18)-C(19)-H(19B)	110.8
H(19A)-C(19)-H(19B)	108.9
N(4)-C(20)-H(20A)	109.5
N(4)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
N(4)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(2)-C(21)-O(1)	125.4(5)
O(2)-C(21)-C(22)	117.1(5)
O(1)-C(21)-C(22)	117.5(5)
C(23)-C(22)-C(24)	125.4(5)
C(23)-C(22)-C(21)	117.6(5)
C(24)-C(22)-C(21)	116.9(5)
C(22)-C(23)-H(23A)	120.0
C(22)-C(23)-H(23B)	120.0
H(23A)-C(23)-H(23B)	120.0
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(4)-C(25)-O(3)	126.0(5)
O(4)-C(25)-C(26)	117.2(4)
O(3)-C(25)-C(26)	116.9(4)
C(28)-C(26)-C(27)	123.4(5)
C(28)-C(26)-C(25)	118.0(4)
C(27)-C(26)-C(25)	118.5(4)
C(26)-C(27)-H(27A)	120.0
C(26)-C(27)-H(27B)	120.0
H(27A)-C(27)-H(27B)	120.0
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(6)-C(29)-O(5)	125.8(5)
O(6)-C(29)-C(30)	117.6(4)
O(5)-C(29)-C(30)	116.6(4)
C(32)-C(30)-C(31)	122.0(5)
C(32)-C(30)-C(29)	119.9(5)

C(31)-C(30)-C(29)	118.2(5)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	120.0
C(30)-C(32)-H(32B)	120.0
H(32A)-C(32)-H(32B)	120.0
O(8)-C(33)-O(7)	125.1(4)
O(8)-C(33)-C(34)	116.4(4)
O(7)-C(33)-C(34)	118.5(4)
C(36)-C(34)-C(35)	123.0(5)
C(36)-C(34)-C(33)	118.9(4)
C(35)-C(34)-C(33)	118.0(4)
C(34)-C(35)-H(35A)	120.0
C(34)-C(35)-H(35B)	120.0
H(35A)-C(35)-H(35B)	120.0
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for CMN. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	25(1)	25(1)	29(1)	7(1)	8(1)	6(1)
Cu(2)	27(1)	24(1)	28(1)	7(1)	9(1)	8(1)
O(1)	27(2)	36(2)	39(2)	14(2)	10(2)	2(2)
O(2)	32(2)	34(2)	38(2)	10(2)	15(2)	2(2)
O(3)	41(2)	29(2)	28(2)	7(2)	11(2)	10(2)
O(4)	37(2)	29(2)	31(2)	7(2)	8(2)	15(2)
O(5)	24(2)	43(2)	39(2)	14(2)	9(2)	6(2)
O(6)	22(2)	33(2)	43(2)	13(2)	10(2)	8(2)
O(7)	40(2)	28(2)	27(2)	4(2)	12(2)	10(2)
O(8)	44(2)	24(2)	30(2)	4(2)	13(2)	11(2)
N(1)	21(2)	19(2)	35(2)	7(2)	6(2)	6(2)
N(2)	29(2)	38(2)	41(2)	13(1)	15(1)	12(1)
N(3)	25(2)	28(2)	27(2)	8(2)	11(2)	8(2)
N(4)	29(2)	26(1)	46(2)	12(1)	16(1)	6(1)
C(1)	23(2)	25(2)	34(2)	11(2)	14(2)	5(2)
C(2)	38(2)	28(2)	36(2)	11(2)	18(2)	7(2)
C(3)	34(2)	29(2)	31(2)	12(2)	9(2)	3(2)
C(4)	23(2)	21(2)	33(2)	5(2)	2(2)	7(2)

C(5)	28(2)	28(2)	32(2)	4(2)	13(2)	7(2)
C(6)	29(2)	29(2)	43(2)	9(2)	12(2)	7(1)
C(7)	38(3)	31(3)	87(4)	13(3)	7(3)	9(2)
C(8)	26(2)	56(3)	92(4)	25(3)	15(2)	8(2)
C(9)	34(2)	50(2)	73(3)	28(2)	30(2)	23(2)
C(10)	43(2)	34(2)	57(3)	7(2)	18(2)	12(2)
C(11)	27(2)	26(2)	41(3)	2(2)	14(2)	10(2)
C(12)	38(3)	35(2)	31(2)	10(2)	20(2)	5(2)
C(13)	41(3)	26(2)	37(2)	14(2)	10(2)	7(2)
C(14)	29(2)	24(2)	31(2)	5(2)	10(2)	5(2)
C(15)	29(2)	25(2)	26(2)	6(2)	6(2)	6(2)
C(16)	26(2)	31(2)	37(2)	16(2)	15(2)	11(2)
C(17)	31(2)	36(3)	79(4)	15(3)	11(2)	4(2)
C(18)	28(2)	52(3)	81(3)	24(2)	11(2)	11(2)
C(19)	29(2)	39(2)	60(2)	27(2)	17(2)	14(2)
C(20)	38(2)	33(2)	77(3)	-5(2)	23(2)	6(2)
C(21)	28(3)	21(3)	42(3)	2(2)	11(3)	7(2)
C(22)	28(3)	31(3)	44(3)	-4(2)	17(2)	-1(2)
C(23)	20(2)	74(4)	42(3)	11(3)	5(2)	-5(3)
C(24)	32(3)	56(4)	53(4)	6(3)	21(3)	-8(3)
C(25)	18(2)	30(3)	28(3)	0(2)	7(2)	-1(2)
C(26)	22(2)	24(3)	36(3)	7(2)	14(2)	6(2)
C(27)	57(3)	27(3)	33(3)	4(2)	20(2)	12(2)
C(28)	38(2)	25(3)	34(3)	0(2)	15(2)	6(2)
C(29)	29(3)	19(3)	32(3)	1(2)	14(2)	5(2)
C(30)	29(3)	33(3)	38(3)	-3(2)	15(2)	2(2)
C(31)	49(4)	74(5)	61(4)	25(4)	28(3)	3(3)
C(32)	32(3)	46(3)	49(3)	2(3)	18(3)	10(2)
C(33)	15(2)	24(3)	35(3)	10(2)	8(2)	3(2)
C(34)	18(2)	24(3)	35(3)	-1(2)	6(2)	-2(2)
C(35)	40(3)	34(3)	34(3)	10(2)	16(2)	13(2)
C(36)	32(3)	35(3)	41(3)	10(2)	13(2)	13(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for CMN.

	x	y	z	U(eq)
H(1)	3014	8316	11111	31
H(2)	3839	7382	12853	39
H(3)	5963	6338	13093	38
H(5)	6272	7193	9814	36
H(6)	7735	5356	12210	40
H(7A)	9081	7973	11806	67
H(7B)	9577	7451	13106	67
H(8A)	11048	6107	12323	70
H(8B)	10711	6790	11115	70
H(9A)	9522	4473	9885	56
H(9B)	9340	4011	11131	56
H(10A)	6719	3181	10424	68
H(10B)	6676	3203	8988	68

H(10C)	5603	4023	9644	68
H(11)	3422	9733	3764	38
H(12)	2280	10713	2101	39
H(13)	164	11689	2163	41
H(15)	425	10554	5419	33
H(16)	-1412	11792	4793	35
H(17A)	-3115	9898	3137	62
H(17B)	-2645	10407	2014	62
H(18A)	-4447	11724	1889	66
H(18B)	-4679	11466	3195	66
H(19A)	-3288	14019	3164	47
H(19B)	-3052	13560	4490	47
H(20A)	-328	14314	5545	79
H(20B)	-513	15275	4547	79
H(20C)	678	14233	4621	79
H(23A)	9746	10885	9342	59
H(23B)	8427	10056	9749	59
H(24A)	9006	11768	7462	74
H(24B)	7323	12009	7028	74
H(24C)	7717	10525	6313	74
H(27A)	4644	3174	5897	46
H(27B)	4657	4397	7222	46
H(28A)	3809	3689	3869	51
H(28B)	4362	5377	4008	51
H(28C)	2639	4751	3756	51
H(31A)	-2284	6581	7941	89
H(31B)	-567	7135	8855	89
H(31C)	-1103	5565	7772	89
H(32A)	-3066	7054	5884	52
H(32B)	-1811	7840	5384	52
H(35A)	2624	14104	11158	42
H(35B)	3122	12532	11203	42
H(36A)	1886	14606	9129	53
H(36B)	1298	13231	7836	53
H(36C)	2984	14130	8335	53

Table 6. Torsion angles [deg] for CMN.

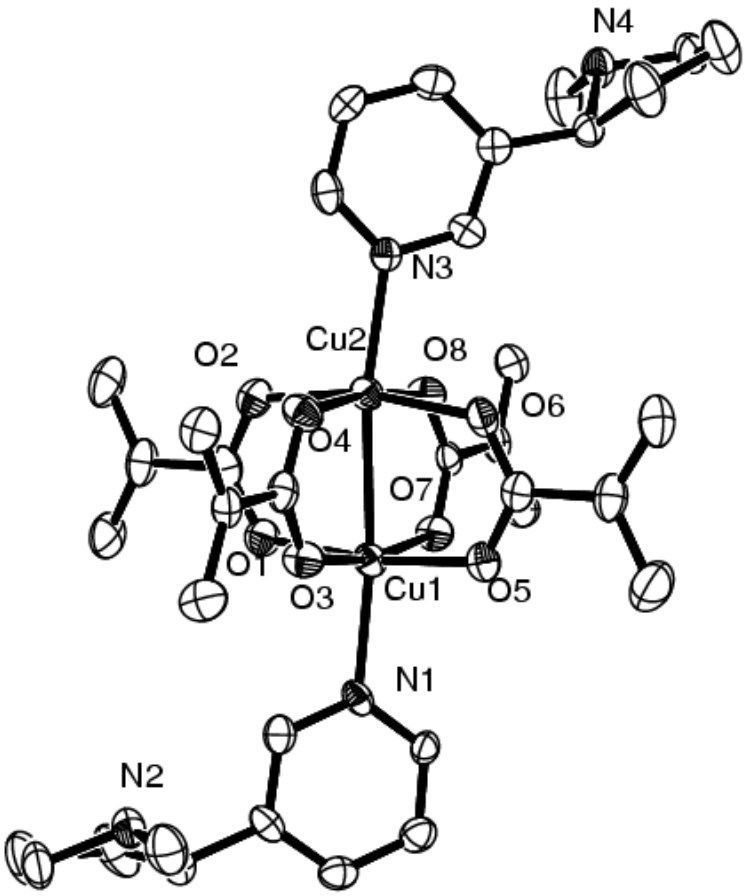
O(1)-Cu(1)-Cu(2)-O(2)	2.88(13)
O(5)-Cu(1)-Cu(2)-O(2)	-178.1(2)
O(7)-Cu(1)-Cu(2)-O(2)	93.65(14)
O(3)-Cu(1)-Cu(2)-O(2)	-87.32(15)
N(1)-Cu(1)-Cu(2)-O(2)	-71.1(7)
O(1)-Cu(1)-Cu(2)-O(4)	91.74(14)
O(5)-Cu(1)-Cu(2)-O(4)	-89.19(15)
O(7)-Cu(1)-Cu(2)-O(4)	-177.49(19)
O(3)-Cu(1)-Cu(2)-O(4)	1.54(13)
N(1)-Cu(1)-Cu(2)-O(4)	17.7(7)
O(1)-Cu(1)-Cu(2)-O(8)	-88.00(15)
O(5)-Cu(1)-Cu(2)-O(8)	91.06(15)
O(7)-Cu(1)-Cu(2)-O(8)	2.76(13)

O(3)-Cu(1)-Cu(2)-O(8)	-178.20(19)
N(1)-Cu(1)-Cu(2)-O(8)	-162.0(7)
O(1)-Cu(1)-Cu(2)-O(6)	-177.80(19)
O(5)-Cu(1)-Cu(2)-O(6)	1.26(12)
O(7)-Cu(1)-Cu(2)-O(6)	-87.04(14)
O(3)-Cu(1)-Cu(2)-O(6)	92.00(14)
N(1)-Cu(1)-Cu(2)-O(6)	108.2(7)
O(1)-Cu(1)-Cu(2)-N(3)	-113.9(6)
O(5)-Cu(1)-Cu(2)-N(3)	65.2(6)
O(7)-Cu(1)-Cu(2)-N(3)	-23.1(6)
O(3)-Cu(1)-Cu(2)-N(3)	155.9(6)
N(1)-Cu(1)-Cu(2)-N(3)	172.1(12)
O(5)-Cu(1)-O(1)-C(21)	-10.3(12)
O(7)-Cu(1)-O(1)-C(21)	-91.4(4)
O(3)-Cu(1)-O(1)-C(21)	75.6(4)
N(1)-Cu(1)-O(1)-C(21)	167.0(4)
Cu(2)-Cu(1)-O(1)-C(21)	-4.7(4)
O(4)-Cu(2)-O(2)-C(21)	-90.9(4)
O(8)-Cu(2)-O(2)-C(21)	79.8(4)
O(6)-Cu(2)-O(2)-C(21)	-5.3(9)
N(3)-Cu(2)-O(2)-C(21)	167.5(4)
Cu(1)-Cu(2)-O(2)-C(21)	-2.2(4)
O(1)-Cu(1)-O(3)-C(25)	-85.1(4)
O(5)-Cu(1)-O(3)-C(25)	85.3(4)
O(7)-Cu(1)-O(3)-C(25)	2.7(10)
N(1)-Cu(1)-O(3)-C(25)	-179.1(4)
Cu(2)-Cu(1)-O(3)-C(25)	-1.5(4)
O(2)-Cu(2)-O(4)-C(25)	83.2(3)
O(8)-Cu(2)-O(4)-C(25)	-0.6(12)
O(6)-Cu(2)-O(4)-C(25)	-84.0(3)
N(3)-Cu(2)-O(4)-C(25)	-177.1(3)
Cu(1)-Cu(2)-O(4)-C(25)	-2.2(3)
O(1)-Cu(1)-O(5)-C(29)	3.0(12)
O(7)-Cu(1)-O(5)-C(29)	84.3(4)
O(3)-Cu(1)-O(5)-C(29)	-82.8(4)
N(1)-Cu(1)-O(5)-C(29)	-174.2(4)
Cu(2)-Cu(1)-O(5)-C(29)	-2.6(3)
O(2)-Cu(2)-O(6)-C(29)	2.7(9)
O(4)-Cu(2)-O(6)-C(29)	88.2(4)
O(8)-Cu(2)-O(6)-C(29)	-82.5(4)
N(3)-Cu(2)-O(6)-C(29)	-170.2(4)
Cu(1)-Cu(2)-O(6)-C(29)	-0.4(3)
O(1)-Cu(1)-O(7)-C(33)	81.5(3)
O(5)-Cu(1)-O(7)-C(33)	-88.9(3)
O(3)-Cu(1)-O(7)-C(33)	-6.1(9)
N(1)-Cu(1)-O(7)-C(33)	175.8(3)
Cu(2)-Cu(1)-O(7)-C(33)	-1.9(3)
O(2)-Cu(2)-O(8)-C(33)	-90.2(4)
O(4)-Cu(2)-O(8)-C(33)	-6.4(12)
O(6)-Cu(2)-O(8)-C(33)	77.0(4)
N(3)-Cu(2)-O(8)-C(33)	170.2(4)
Cu(1)-Cu(2)-O(8)-C(33)	-4.9(4)
O(1)-Cu(1)-N(1)-C(1)	139.0(4)
O(5)-Cu(1)-N(1)-C(1)	-41.4(4)
O(7)-Cu(1)-N(1)-C(1)	47.8(4)
O(3)-Cu(1)-N(1)-C(1)	-131.8(4)
Cu(2)-Cu(1)-N(1)-C(1)	-147.7(5)

O(1)-Cu(1)-N(1)-C(5)	-45.0(4)
O(5)-Cu(1)-N(1)-C(5)	134.6(4)
O(7)-Cu(1)-N(1)-C(5)	-136.2(4)
O(3)-Cu(1)-N(1)-C(5)	44.2(4)
Cu(2)-Cu(1)-N(1)-C(5)	28.3(10)
O(2)-Cu(2)-N(3)-C(11)	39.5(5)
O(4)-Cu(2)-N(3)-C(11)	-51.2(5)
O(8)-Cu(2)-N(3)-C(11)	129.4(4)
O(6)-Cu(2)-N(3)-C(11)	-142.1(4)
Cu(1)-Cu(2)-N(3)-C(11)	155.0(4)
O(2)-Cu(2)-N(3)-C(15)	-137.5(4)
O(4)-Cu(2)-N(3)-C(15)	131.8(4)
O(8)-Cu(2)-N(3)-C(15)	-47.7(4)
O(6)-Cu(2)-N(3)-C(15)	40.9(4)
Cu(1)-Cu(2)-N(3)-C(15)	-22.0(8)
C(5)-N(1)-C(1)-C(2)	0.8(7)
Cu(1)-N(1)-C(1)-C(2)	176.8(3)
N(1)-C(1)-C(2)-C(3)	-0.1(7)
C(1)-C(2)-C(3)-C(4)	-0.6(7)
C(2)-C(3)-C(4)-C(5)	0.6(7)
C(2)-C(3)-C(4)-C(6)	179.9(4)
C(1)-N(1)-C(5)-C(4)	-0.9(7)
Cu(1)-N(1)-C(5)-C(4)	-177.0(3)
C(3)-C(4)-C(5)-N(1)	0.2(7)
C(6)-C(4)-C(5)-N(1)	-179.2(4)
C(10)-N(2)-C(6)-C(4)	-68.2(4)
C(9)-N(2)-C(6)-C(4)	169.8(3)
C(10)-N(2)-C(6)-C(7)	168.2(3)
C(9)-N(2)-C(6)-C(7)	46.1(4)
C(3)-C(4)-C(6)-N(2)	139.4(4)
C(5)-C(4)-C(6)-N(2)	-41.3(5)
C(3)-C(4)-C(6)-C(7)	-103.4(5)
C(5)-C(4)-C(6)-C(7)	76.0(5)
N(2)-C(6)-C(7)-C(8)	-32.0(5)
C(4)-C(6)-C(7)-C(8)	-154.9(4)
C(6)-C(7)-C(8)-C(9)	6.6(5)
C(10)-N(2)-C(9)-C(8)	-164.4(3)
C(6)-N(2)-C(9)-C(8)	-41.7(4)
C(7)-C(8)-C(9)-N(2)	20.4(5)
C(15)-N(3)-C(11)-C(12)	-0.7(7)
Cu(2)-N(3)-C(11)-C(12)	-177.6(3)
N(3)-C(11)-C(12)-C(13)	1.1(7)
C(11)-C(12)-C(13)-C(14)	-1.0(7)
C(12)-C(13)-C(14)-C(15)	0.5(7)
C(12)-C(13)-C(14)-C(16)	-176.7(4)
C(11)-N(3)-C(15)-C(14)	0.2(7)
Cu(2)-N(3)-C(15)-C(14)	177.6(4)
C(13)-C(14)-C(15)-N(3)	-0.1(7)
C(16)-C(14)-C(15)-N(3)	177.3(4)
C(20)-N(4)-C(16)-C(14)	-66.0(4)
C(19)-N(4)-C(16)-C(14)	171.0(3)
C(20)-N(4)-C(16)-C(17)	170.9(4)
C(19)-N(4)-C(16)-C(17)	47.9(4)
C(13)-C(14)-C(16)-N(4)	-45.9(6)
C(15)-C(14)-C(16)-N(4)	136.9(4)
C(13)-C(14)-C(16)-C(17)	70.4(6)
C(15)-C(14)-C(16)-C(17)	-106.8(5)

N(4)-C(16)-C(17)-C(18)	-35.6(5)
C(14)-C(16)-C(17)-C(18)	-158.6(4)
C(16)-C(17)-C(18)-C(19)	10.5(5)
C(16)-N(4)-C(19)-C(18)	-41.5(4)
C(20)-N(4)-C(19)-C(18)	-164.3(3)
C(17)-C(18)-C(19)-N(4)	18.0(5)
Cu(2)-O(2)-C(21)-O(1)	-0.6(7)
Cu(2)-O(2)-C(21)-C(22)	179.2(3)
Cu(1)-O(1)-C(21)-O(2)	4.7(7)
Cu(1)-O(1)-C(21)-C(22)	-175.2(3)
O(2)-C(21)-C(22)-C(23)	-173.6(5)
O(1)-C(21)-C(22)-C(23)	6.2(7)
O(2)-C(21)-C(22)-C(24)	7.0(7)
O(1)-C(21)-C(22)-C(24)	-173.1(5)
Cu(2)-O(4)-C(25)-O(3)	1.8(6)
Cu(2)-O(4)-C(25)-C(26)	-177.5(3)
Cu(1)-O(3)-C(25)-O(4)	0.3(7)
Cu(1)-O(3)-C(25)-C(26)	179.6(3)
O(4)-C(25)-C(26)-C(28)	0.0(6)
O(3)-C(25)-C(26)-C(28)	-179.3(5)
O(4)-C(25)-C(26)-C(27)	-179.2(4)
O(3)-C(25)-C(26)-C(27)	1.4(6)
Cu(2)-O(6)-C(29)-O(5)	-1.6(7)
Cu(2)-O(6)-C(29)-C(30)	177.3(3)
Cu(1)-O(5)-C(29)-O(6)	3.2(7)
Cu(1)-O(5)-C(29)-C(30)	-175.7(3)
O(6)-C(29)-C(30)-C(32)	-4.7(7)
O(5)-C(29)-C(30)-C(32)	174.3(5)
O(6)-C(29)-C(30)-C(31)	176.7(5)
O(5)-C(29)-C(30)-C(31)	-4.3(7)
Cu(2)-O(8)-C(33)-O(7)	5.1(7)
Cu(2)-O(8)-C(33)-C(34)	-175.1(3)
Cu(1)-O(7)-C(33)-O(8)	-1.1(6)
Cu(1)-O(7)-C(33)-C(34)	179.2(3)
O(8)-C(33)-C(34)-C(36)	0.0(6)
O(7)-C(33)-C(34)-C(36)	179.7(4)
O(8)-C(33)-C(34)-C(35)	-179.9(5)
O(7)-C(33)-C(34)-C(35)	-0.1(6)

Symmetry transformations used to generate equivalent atoms:



Crystal structure of CMN

Crystallographic details of ZMS 59

Table 1. Crystal data and structure refinement for ZMS.

Identification code	ZMS
Empirical formula	C23 H36 N2 O4 Zn
Formula weight	469.91
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21
Unit cell dimensions	a = 14.1674(2) A alpha = 90 deg. b = 11.4910(2) A beta = 113.205(1) deg. c = 14.8774(3) A gamma = 90 deg.
Volume	2226.07(7) A^3
Z, Calculated density	4, 1.402 Mg/m^3
Absorption coefficient	1.135 mm^-1
F(000)	1000
Crystal size	0.30 x 0.20 x 0.15 mm
Theta range for data collection	1.49 to 27.51 deg.
Limiting indices	-18<=h<=18, -14<=k<=14, -19<=l<=19
Reflections collected / unique	41630 / 10225 [R(int) = 0.099]
Completeness to theta = 27.51	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10225 / 1 / 546
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.0951
R indices (all data)	R1 = 0.0693, wR2 = 0.1044
Absolute structure parameter	0.026(11)
Largest diff. peak and hole	0.616 and -0.543 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ZMS. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	2845(1)	1109(1)	650(1)	21(1)
Zn(2)	2302(1)	6619(1)	4458(1)	22(1)
O(1)	2542(2)	2126(3)	-470(2)	31(1)
O(2)	3566(2)	1174(3)	-1030(2)	41(1)
O(3)	1620(2)	123(3)	457(2)	32(1)
O(4)	1261(2)	1794(3)	944(2)	42(1)
O(5)	3530(2)	5828(2)	4432(2)	31(1)
O(6)	3974(3)	7664(3)	4501(3)	44(1)
O(7)	2532(2)	7345(3)	5684(2)	32(1)
O(8)	1517(3)	6211(3)	6117(2)	50(1)
N(1)	3861(2)	-326(3)	1026(2)	22(1)
N(2)	3767(2)	1865(3)	1999(2)	24(1)
N(3)	1285(2)	5223(3)	3872(2)	21(1)
N(4)	1439(2)	7611(3)	3229(2)	23(1)
C(1)	3457(3)	-1129(3)	164(3)	26(1)
C(2)	3907(3)	-2352(4)	363(3)	32(1)
C(3)	3712(3)	-2886(4)	1215(3)	36(1)
C(4)	4183(3)	-2122(4)	2106(3)	32(1)
C(5)	3762(3)	-868(3)	1909(3)	25(1)
C(6)	4262(3)	-108(4)	2815(3)	26(1)
C(7)	3714(3)	1057(4)	2765(3)	28(1)
C(8)	4868(3)	2002(3)	2111(3)	25(1)
C(9)	5380(3)	823(4)	2131(3)	26(1)
C(10)	4925(3)	68(4)	1214(3)	24(1)
C(11)	5385(3)	144(4)	3010(3)	31(1)
C(12)	3370(3)	3017(4)	2149(3)	29(1)
C(13)	3395(3)	3904(4)	1403(3)	32(1)
C(14)	4466(3)	4020(4)	1413(4)	36(1)
C(15)	4907(3)	2832(4)	1333(3)	29(1)
C(16)	2971(3)	1972(4)	-1079(3)	28(1)
C(17)	2710(3)	2860(4)	-1888(3)	29(1)
C(18)	2323(3)	3979(4)	-1754(4)	42(1)
C(19)	2873(3)	2567(4)	-2719(3)	41(1)
C(20)	1011(3)	785(4)	648(3)	25(1)
C(21)	-21(3)	315(4)	532(3)	28(1)
C(22)	-740(3)	1148(5)	692(4)	45(1)
C(23)	-252(3)	-793(4)	286(3)	35(1)
C(24)	1631(3)	4260(3)	4606(3)	26(1)
C(25)	1132(3)	3088(3)	4248(3)	29(1)
C(26)	1290(3)	2736(4)	3327(3)	31(1)
C(27)	891(3)	3675(3)	2558(3)	28(1)
C(28)	1394(3)	4852(4)	2937(3)	24(1)
C(29)	970(3)	5804(3)	2148(3)	27(1)
C(30)	1537(3)	6963(4)	2391(3)	29(1)
C(31)	329(3)	7708(4)	3075(3)	27(1)
C(32)	-200(3)	6501(4)	2875(3)	28(1)
C(33)	213(3)	5601(4)	3685(3)	25(1)
C(34)	-165(3)	6031(4)	1923(3)	30(1)
C(35)	1847(3)	8812(4)	3252(3)	29(1)
C(36)	1780(3)	9519(4)	4079(3)	33(1)

C(37)	678(3)	9577(4)	4013(4)	38(1)
C(38)	222(3)	8360(4)	3917(3)	31(1)
C(39)	4174(3)	6629(5)	4477(3)	28(1)
C(40)	5204(3)	6258(4)	4491(3)	32(1)
C(41)	5958(3)	7162(5)	4647(3)	43(1)
C(42)	5356(4)	5120(5)	4360(4)	55(2)
C(43)	2050(3)	7072(4)	6231(3)	27(1)
C(44)	2152(3)	7924(4)	7032(3)	29(1)
C(45)	1783(3)	7556(4)	7745(3)	40(1)
C(46)	2583(4)	9028(4)	7038(4)	44(1)

Table 3. Bond lengths [A] and angles [deg] for ZMS.

Zn(1)-O(1)	1.939(3)
Zn(1)-O(3)	1.996(3)
Zn(1)-N(2)	2.104(3)
Zn(1)-N(1)	2.114(3)
Zn(2)-O(7)	1.913(3)
Zn(2)-O(5)	1.977(3)
Zn(2)-N(4)	2.092(3)
Zn(2)-N(3)	2.102(3)
O(1)-C(16)	1.288(5)
O(2)-C(16)	1.228(5)
O(3)-C(20)	1.264(5)
O(4)-C(20)	1.241(5)
O(5)-C(39)	1.280(5)
O(6)-C(39)	1.226(6)
O(7)-C(43)	1.291(5)
O(8)-C(43)	1.216(5)
N(1)-C(10)	1.491(5)
N(1)-C(1)	1.498(5)
N(1)-C(5)	1.509(5)
N(2)-C(12)	1.489(5)
N(2)-C(7)	1.495(5)
N(2)-C(8)	1.509(5)
N(3)-C(24)	1.496(5)
N(3)-C(33)	1.497(4)
N(3)-C(28)	1.519(5)
N(4)-C(35)	1.491(5)
N(4)-C(31)	1.502(5)
N(4)-C(30)	1.506(5)
C(1)-C(2)	1.524(6)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.527(6)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.509(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.543(6)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900

C(5)-C(6)	1.526(6)
C(5)-H(5)	1.0000
C(6)-C(11)	1.528(5)
C(6)-C(7)	1.534(6)
C(6)-H(6)	1.0000
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(15)	1.518(6)
C(8)-C(9)	1.532(5)
C(8)-H(8)	1.0000
C(9)-C(11)	1.521(6)
C(9)-C(10)	1.528(5)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.517(6)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.518(6)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.525(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.508(6)
C(17)-C(19)	1.385(6)
C(17)-C(18)	1.442(6)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9500
C(19)-H(19B)	0.9500
C(20)-C(21)	1.503(5)
C(21)-C(23)	1.330(6)
C(21)-C(22)	1.485(6)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9500
C(23)-H(23B)	0.9500
C(24)-C(25)	1.516(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.527(6)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.511(6)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.529(6)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.543(6)

C(28)-H(28)	1.0000
C(29)-C(30)	1.524(6)
C(29)-C(34)	1.529(5)
C(29)-H(29)	1.0000
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(38)	1.517(6)
C(31)-C(32)	1.549(6)
C(31)-H(31)	1.0000
C(32)-C(33)	1.520(6)
C(32)-C(34)	1.535(6)
C(32)-H(32)	1.0000
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.509(6)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-C(37)	1.526(6)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.524(6)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.513(5)
C(40)-C(42)	1.351(7)
C(40)-C(41)	1.442(6)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9500
C(42)-H(42B)	0.9500
C(43)-C(44)	1.504(5)
C(44)-C(46)	1.406(6)
C(44)-C(45)	1.421(6)
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9500
C(46)-H(46B)	0.9500

O(1)-Zn(1)-O(3)	109.47(12)
O(1)-Zn(1)-N(2)	114.48(12)
O(3)-Zn(1)-N(2)	123.36(12)
O(1)-Zn(1)-N(1)	126.47(12)
O(3)-Zn(1)-N(1)	93.32(12)
N(2)-Zn(1)-N(1)	88.11(12)
O(7)-Zn(2)-O(5)	113.51(12)
O(7)-Zn(2)-N(4)	114.63(13)
O(5)-Zn(2)-N(4)	116.69(12)
O(7)-Zn(2)-N(3)	124.06(12)
O(5)-Zn(2)-N(3)	96.03(12)
N(4)-Zn(2)-N(3)	89.09(12)
C(16)-O(1)-Zn(1)	121.1(3)

C(20)-O(3)-Zn(1)	104.9(3)
C(39)-O(5)-Zn(2)	106.4(3)
C(43)-O(7)-Zn(2)	124.2(3)
C(10)-N(1)-C(1)	111.4(3)
C(10)-N(1)-C(5)	113.3(3)
C(1)-N(1)-C(5)	110.9(3)
C(10)-N(1)-Zn(1)	110.2(2)
C(1)-N(1)-Zn(1)	105.3(2)
C(5)-N(1)-Zn(1)	105.4(2)
C(12)-N(2)-C(7)	107.6(3)
C(12)-N(2)-C(8)	109.0(3)
C(7)-N(2)-C(8)	109.9(3)
C(12)-N(2)-Zn(1)	112.4(2)
C(7)-N(2)-Zn(1)	105.7(2)
C(8)-N(2)-Zn(1)	112.0(2)
C(24)-N(3)-C(33)	111.5(3)
C(24)-N(3)-C(28)	109.8(3)
C(33)-N(3)-C(28)	111.9(3)
C(24)-N(3)-Zn(2)	106.8(2)
C(33)-N(3)-Zn(2)	109.6(2)
C(28)-N(3)-Zn(2)	107.1(2)
C(35)-N(4)-C(31)	108.0(3)
C(35)-N(4)-C(30)	108.4(3)
C(31)-N(4)-C(30)	110.1(3)
C(35)-N(4)-Zn(2)	113.4(2)
C(31)-N(4)-Zn(2)	113.0(2)
C(30)-N(4)-Zn(2)	104.0(2)
N(1)-C(1)-C(2)	114.4(3)
N(1)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1A)	108.7
N(1)-C(1)-H(1B)	108.7
C(2)-C(1)-H(1B)	108.7
H(1A)-C(1)-H(1B)	107.6
C(1)-C(2)-C(3)	109.5(3)
C(1)-C(2)-H(2A)	109.8
C(3)-C(2)-H(2A)	109.8
C(1)-C(2)-H(2B)	109.8
C(3)-C(2)-H(2B)	109.8
H(2A)-C(2)-H(2B)	108.2
C(4)-C(3)-C(2)	109.5(4)
C(4)-C(3)-H(3A)	109.8
C(2)-C(3)-H(3A)	109.8
C(4)-C(3)-H(3B)	109.8
C(2)-C(3)-H(3B)	109.8
H(3A)-C(3)-H(3B)	108.2
C(3)-C(4)-C(5)	111.8(3)
C(3)-C(4)-H(4A)	109.2
C(5)-C(4)-H(4A)	109.2
C(3)-C(4)-H(4B)	109.2
C(5)-C(4)-H(4B)	109.2
H(4A)-C(4)-H(4B)	107.9
N(1)-C(5)-C(6)	111.3(3)
N(1)-C(5)-C(4)	112.9(3)
C(6)-C(5)-C(4)	110.9(3)
N(1)-C(5)-H(5)	107.2
C(6)-C(5)-H(5)	107.2
C(4)-C(5)-H(5)	107.2

C(5)-C(6)-C(11)	111.3(3)
C(5)-C(6)-C(7)	114.0(3)
C(11)-C(6)-C(7)	108.3(3)
C(5)-C(6)-H(6)	107.7
C(11)-C(6)-H(6)	107.7
C(7)-C(6)-H(6)	107.7
N(2)-C(7)-C(6)	113.7(3)
N(2)-C(7)-H(7A)	108.8
C(6)-C(7)-H(7A)	108.8
N(2)-C(7)-H(7B)	108.8
C(6)-C(7)-H(7B)	108.8
H(7A)-C(7)-H(7B)	107.7
N(2)-C(8)-C(15)	109.1(3)
N(2)-C(8)-C(9)	111.8(3)
C(15)-C(8)-C(9)	114.3(3)
N(2)-C(8)-H(8)	107.1
C(15)-C(8)-H(8)	107.1
C(9)-C(8)-H(8)	107.1
C(11)-C(9)-C(10)	109.5(3)
C(11)-C(9)-C(8)	108.2(3)
C(10)-C(9)-C(8)	117.0(3)
C(11)-C(9)-H(9)	107.2
C(10)-C(9)-H(9)	107.2
C(8)-C(9)-H(9)	107.2
N(1)-C(10)-C(9)	112.3(3)
N(1)-C(10)-H(10A)	109.1
C(9)-C(10)-H(10A)	109.1
N(1)-C(10)-H(10B)	109.1
C(9)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.9
C(9)-C(11)-C(6)	106.3(3)
C(9)-C(11)-H(11A)	110.5
C(6)-C(11)-H(11A)	110.5
C(9)-C(11)-H(11B)	110.5
C(6)-C(11)-H(11B)	110.5
H(11A)-C(11)-H(11B)	108.7
N(2)-C(12)-C(13)	111.6(3)
N(2)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12A)	109.3
N(2)-C(12)-H(12B)	109.3
C(13)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-C(14)	111.3(4)
C(12)-C(13)-H(13A)	109.4
C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13B)	109.4
C(14)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(15)	111.1(4)
C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14B)	109.4
C(15)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
C(8)-C(15)-C(14)	111.3(3)
C(8)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15A)	109.4

C(8)-C(15)-H(15B)	109.4
C(14)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
O(2)-C(16)-O(1)	124.4(4)
O(2)-C(16)-C(17)	119.9(4)
O(1)-C(16)-C(17)	115.7(4)
C(19)-C(17)-C(18)	123.1(4)
C(19)-C(17)-C(16)	118.2(4)
C(18)-C(17)-C(16)	118.7(4)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	120.0
C(17)-C(19)-H(19B)	120.0
H(19A)-C(19)-H(19B)	120.0
O(4)-C(20)-O(3)	121.2(4)
O(4)-C(20)-C(21)	120.4(4)
O(3)-C(20)-C(21)	118.5(4)
C(23)-C(21)-C(22)	123.4(4)
C(23)-C(21)-C(20)	119.9(4)
C(22)-C(21)-C(20)	116.6(4)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	120.0
C(21)-C(23)-H(23B)	120.0
H(23A)-C(23)-H(23B)	120.0
N(3)-C(24)-C(25)	115.3(3)
N(3)-C(24)-H(24A)	108.4
C(25)-C(24)-H(24A)	108.4
N(3)-C(24)-H(24B)	108.4
C(25)-C(24)-H(24B)	108.4
H(24A)-C(24)-H(24B)	107.5
C(24)-C(25)-C(26)	109.7(3)
C(24)-C(25)-H(25A)	109.7
C(26)-C(25)-H(25A)	109.7
C(24)-C(25)-H(25B)	109.7
C(26)-C(25)-H(25B)	109.7
H(25A)-C(25)-H(25B)	108.2
C(27)-C(26)-C(25)	110.3(3)
C(27)-C(26)-H(26A)	109.6
C(25)-C(26)-H(26A)	109.6
C(27)-C(26)-H(26B)	109.6
C(25)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	108.1
C(26)-C(27)-C(28)	111.8(3)
C(26)-C(27)-H(27A)	109.3
C(28)-C(27)-H(27A)	109.3
C(26)-C(27)-H(27B)	109.3
C(28)-C(27)-H(27B)	109.3
H(27A)-C(27)-H(27B)	107.9

N(3)-C(28)-C(27)	112.6(3)
N(3)-C(28)-C(29)	110.3(3)
C(27)-C(28)-C(29)	111.2(3)
N(3)-C(28)-H(28)	107.5
C(27)-C(28)-H(28)	107.5
C(29)-C(28)-H(28)	107.5
C(30)-C(29)-C(34)	108.3(3)
C(30)-C(29)-C(28)	115.4(3)
C(34)-C(29)-C(28)	110.4(3)
C(30)-C(29)-H(29)	107.5
C(34)-C(29)-H(29)	107.5
C(28)-C(29)-H(29)	107.5
N(4)-C(30)-C(29)	114.6(3)
N(4)-C(30)-H(30A)	108.6
C(29)-C(30)-H(30A)	108.6
N(4)-C(30)-H(30B)	108.6
C(29)-C(30)-H(30B)	108.6
H(30A)-C(30)-H(30B)	107.6
N(4)-C(31)-C(38)	110.5(3)
N(4)-C(31)-C(32)	111.2(3)
C(38)-C(31)-C(32)	113.7(3)
N(4)-C(31)-H(31)	107.0
C(38)-C(31)-H(31)	107.0
C(32)-C(31)-H(31)	107.0
C(33)-C(32)-C(34)	110.5(4)
C(33)-C(32)-C(31)	116.8(3)
C(34)-C(32)-C(31)	107.7(3)
C(33)-C(32)-H(32)	107.1
C(34)-C(32)-H(32)	107.1
C(31)-C(32)-H(32)	107.1
N(3)-C(33)-C(32)	112.9(3)
N(3)-C(33)-H(33A)	109.0
C(32)-C(33)-H(33A)	109.0
N(3)-C(33)-H(33B)	109.0
C(32)-C(33)-H(33B)	109.0
H(33A)-C(33)-H(33B)	107.8
C(29)-C(34)-C(32)	105.7(3)
C(29)-C(34)-H(34A)	110.6
C(32)-C(34)-H(34A)	110.6
C(29)-C(34)-H(34B)	110.6
C(32)-C(34)-H(34B)	110.6
H(34A)-C(34)-H(34B)	108.7
N(4)-C(35)-C(36)	111.6(3)
N(4)-C(35)-H(35A)	109.3
C(36)-C(35)-H(35A)	109.3
N(4)-C(35)-H(35B)	109.3
C(36)-C(35)-H(35B)	109.3
H(35A)-C(35)-H(35B)	108.0
C(35)-C(36)-C(37)	111.3(4)
C(35)-C(36)-H(36A)	109.4
C(37)-C(36)-H(36A)	109.4
C(35)-C(36)-H(36B)	109.4
C(37)-C(36)-H(36B)	109.4
H(36A)-C(36)-H(36B)	108.0
C(38)-C(37)-C(36)	110.5(4)
C(38)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37A)	109.5

C(38)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	108.1
C(31)-C(38)-C(37)	110.7(4)
C(31)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38A)	109.5
C(31)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	108.1
O(6)-C(39)-O(5)	122.0(4)
O(6)-C(39)-C(40)	120.4(4)
O(5)-C(39)-C(40)	117.5(4)
C(42)-C(40)-C(41)	124.8(4)
C(42)-C(40)-C(39)	118.6(4)
C(41)-C(40)-C(39)	116.7(4)
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	120.0
C(40)-C(42)-H(42B)	120.0
H(42A)-C(42)-H(42B)	120.0
O(8)-C(43)-O(7)	124.3(4)
O(8)-C(43)-C(44)	120.1(4)
O(7)-C(43)-C(44)	115.5(4)
C(46)-C(44)-C(45)	123.4(4)
C(46)-C(44)-C(43)	119.9(4)
C(45)-C(44)-C(43)	116.7(4)
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-H(46A)	120.0
C(44)-C(46)-H(46B)	120.0
H(46A)-C(46)-H(46B)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ZMS. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	23(1)	22(1)	20(1)	0(1)	8(1)	0(1)
Zn(2)	22(1)	24(1)	19(1)	1(1)	8(1)	1(1)
O(1)	32(2)	36(2)	25(2)	6(1)	12(1)	-2(1)
O(2)	52(2)	40(2)	36(2)	7(2)	21(1)	12(2)

O(3)	22(1)	34(2)	40(2)	5(1)	11(1)	4(1)
O(4)	42(2)	36(2)	49(2)	-12(2)	18(1)	-11(2)
O(5)	22(1)	34(2)	33(2)	-5(1)	9(1)	0(1)
O(6)	45(2)	35(2)	52(2)	11(2)	19(2)	5(2)
O(7)	34(2)	42(2)	21(2)	-4(1)	13(1)	-1(1)
O(8)	67(2)	49(2)	45(2)	-20(2)	34(2)	-26(2)
N(1)	25(2)	22(2)	20(2)	-1(1)	9(1)	2(1)
N(2)	22(2)	27(2)	24(2)	-1(1)	10(1)	0(1)
N(3)	21(2)	22(2)	18(2)	-1(1)	5(1)	1(1)
N(4)	22(2)	25(2)	24(2)	3(1)	10(1)	5(1)
C(1)	29(2)	26(2)	22(2)	-4(2)	11(2)	1(2)
C(2)	40(2)	26(2)	33(2)	-7(2)	18(2)	1(2)
C(3)	41(2)	21(2)	51(3)	3(2)	24(2)	4(2)
C(4)	34(2)	31(2)	32(2)	9(2)	15(2)	2(2)
C(5)	23(2)	29(2)	25(2)	5(2)	11(2)	5(2)
C(6)	29(2)	31(2)	17(2)	3(2)	7(2)	2(2)
C(7)	32(2)	34(2)	18(2)	-1(2)	11(2)	-1(2)
C(8)	23(2)	27(2)	28(2)	-4(2)	13(2)	-4(2)
C(9)	20(2)	32(3)	29(2)	0(2)	11(2)	-1(2)
C(10)	22(2)	25(2)	24(2)	2(2)	8(2)	3(2)
C(11)	28(2)	37(2)	23(2)	3(2)	4(2)	3(2)
C(12)	28(2)	26(2)	38(3)	-10(2)	17(2)	-2(2)
C(13)	34(2)	22(2)	41(3)	0(2)	17(2)	2(2)
C(14)	41(2)	29(2)	41(3)	-2(2)	19(2)	-8(2)
C(15)	24(2)	32(2)	34(2)	0(2)	15(2)	1(2)
C(16)	27(2)	32(2)	21(2)	1(2)	4(2)	-4(2)
C(17)	28(2)	33(2)	25(2)	5(2)	7(2)	-7(2)
C(18)	35(2)	38(3)	44(3)	12(2)	8(2)	-4(2)
C(19)	40(3)	47(3)	35(3)	18(2)	15(2)	-1(2)
C(20)	24(2)	30(2)	20(2)	3(2)	7(2)	-1(2)
C(21)	23(2)	37(2)	22(2)	4(2)	6(2)	1(2)
C(22)	35(2)	49(3)	59(3)	-12(3)	24(2)	-4(2)
C(23)	28(2)	36(3)	35(2)	-1(2)	7(2)	-8(2)
C(24)	28(2)	28(2)	21(2)	1(2)	8(2)	4(2)
C(25)	31(2)	25(2)	29(2)	3(2)	11(2)	0(2)
C(26)	27(2)	27(2)	33(2)	-3(2)	6(2)	3(2)
C(27)	28(2)	30(2)	23(2)	-4(2)	7(2)	5(2)
C(28)	22(2)	29(2)	19(2)	-2(2)	6(2)	5(2)
C(29)	29(2)	33(2)	19(2)	-1(2)	10(2)	5(2)
C(30)	28(2)	39(3)	20(2)	5(2)	10(2)	2(2)
C(31)	22(2)	33(2)	25(2)	2(2)	7(2)	6(2)
C(32)	18(2)	33(3)	28(2)	-1(2)	5(2)	4(2)
C(33)	20(2)	23(2)	33(2)	-1(2)	12(2)	-1(2)
C(34)	27(2)	30(2)	25(2)	0(2)	3(2)	4(2)
C(35)	28(2)	27(2)	31(2)	9(2)	11(2)	4(2)
C(36)	34(2)	21(2)	41(3)	5(2)	11(2)	1(2)
C(37)	36(2)	33(3)	45(3)	-2(2)	17(2)	6(2)
C(38)	27(2)	31(2)	36(2)	0(2)	14(2)	4(2)
C(39)	25(2)	42(3)	17(2)	4(2)	10(1)	2(2)
C(40)	23(2)	56(3)	17(2)	3(2)	6(1)	6(2)
C(41)	28(2)	66(3)	30(2)	10(2)	7(2)	-11(2)
C(42)	28(2)	64(4)	69(4)	-19(3)	16(2)	7(2)
C(43)	26(2)	29(2)	22(2)	-3(2)	5(2)	0(2)
C(44)	25(2)	35(2)	23(2)	-3(2)	6(2)	3(2)
C(45)	35(2)	54(3)	26(2)	-9(2)	7(2)	6(2)
C(46)	49(3)	42(3)	39(3)	-17(2)	15(2)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ZMS.

	x	y	z	U(eq)
H(1A)	3604	-786	-378	31
H(1B)	2702	-1184	-56	31
H(2A)	4655	-2320	526	38
H(2B)	3584	-2840	-228	38
H(3A)	2964	-2958	1038	43
H(3B)	4018	-3673	1358	43
H(4A)	4938	-2104	2309	38
H(4B)	4037	-2458	2651	38
H(5)	3012	-909	1770	30
H(6)	4247	-550	3388	32
H(7A)	2983	902	2632	33
H(7B)	4024	1444	3410	33
H(8)	5249	2380	2759	30
H(9)	6112	979	2243	32
H(10A)	4916	517	644	29
H(10B)	5368	-622	1289	29
H(11A)	5709	607	3616	37
H(11B)	5772	-592	3085	37
H(12A)	3791	3303	2815	35
H(12B)	2655	2927	2096	35
H(13A)	3167	4669	1550	38
H(13B)	2912	3664	743	38
H(14A)	4921	4403	2027	43
H(14B)	4440	4516	859	43
H(15A)	4511	2500	677	35
H(15B)	5628	2925	1405	35
H(18A)	2169	4452	-2343	62
H(18B)	2841	4374	-1192	62
H(18C)	1695	3870	-1635	62
H(19A)	2728	3116	-3234	49
H(19B)	3129	1819	-2773	49
H(22A)	-1398	760	561	68
H(22B)	-851	1813	250	68
H(22C)	-448	1420	1371	68
H(23A)	-907	-1089	204	41
H(23B)	238	-1289	192	41
H(24A)	1490	4489	5183	32
H(24B)	2383	4171	4825	32
H(25A)	389	3134	4103	34
H(25B)	1440	2495	4764	34
H(26A)	2031	2608	3490	37
H(26B)	923	1998	3069	37
H(27A)	138	3747	2352	33
H(27B)	1027	3450	1978	33
H(28)	2144	4770	3090	29
H(29)	1016	5502	1536	32
H(30A)	2275	6819	2549	35
H(30B)	1274	7464	1802	35
H(31)	-17	8189	2474	33
H(32)	-939	6630	2751	33
H(33A)	200	5932	4295	30

H(33B)	-243	4912	3508	30
H(34A)	-567	5302	1723	35
H(34B)	-450	6609	1390	35
H(35A)	1452	9205	2623	35
H(35B)	2573	8767	3329	35
H(36A)	2033	10317	4058	40
H(36B)	2224	9164	4711	40
H(37A)	669	9958	4606	45
H(37B)	257	10051	3439	45
H(38A)	578	7924	4533	37
H(38B)	-514	8417	3804	37
H(41A)	6605	6816	4686	64
H(41B)	6071	7571	5259	64
H(41C)	5711	7714	4101	64
H(42A)	5997	4868	4366	66
H(42B)	4822	4573	4261	66
H(45A)	1831	8202	8191	59
H(45B)	2198	6902	8117	59
H(45C)	1065	7311	7420	59
H(46A)	2639	9571	7538	53
H(46B)	2819	9230	6543	53

Table 6. Torsion angles [deg] for ZMS.

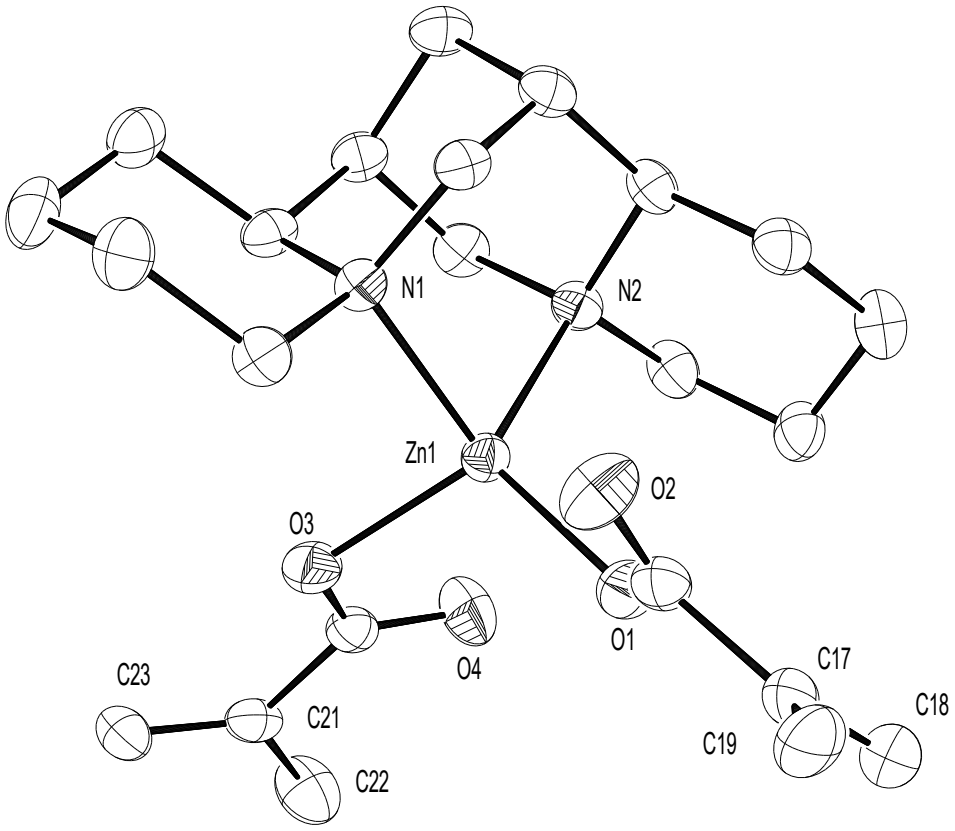
O(3)-Zn(1)-O(1)-C(16)	-109.8(3)
N(2)-Zn(1)-O(1)-C(16)	106.9(3)
N(1)-Zn(1)-O(1)-C(16)	0.0(3)
O(1)-Zn(1)-O(3)-C(20)	-77.6(3)
N(2)-Zn(1)-O(3)-C(20)	61.7(3)
N(1)-Zn(1)-O(3)-C(20)	151.7(3)
O(7)-Zn(2)-O(5)-C(39)	-68.2(3)
N(4)-Zn(2)-O(5)-C(39)	68.5(3)
N(3)-Zn(2)-O(5)-C(39)	160.5(2)
O(5)-Zn(2)-O(7)-C(43)	-118.8(3)
N(4)-Zn(2)-O(7)-C(43)	103.6(3)
N(3)-Zn(2)-O(7)-C(43)	-3.1(4)
O(1)-Zn(1)-N(1)-C(10)	61.3(3)
O(3)-Zn(1)-N(1)-C(10)	178.6(2)
N(2)-Zn(1)-N(1)-C(10)	-58.1(2)
O(1)-Zn(1)-N(1)-C(1)	-58.9(3)
O(3)-Zn(1)-N(1)-C(1)	58.4(2)
N(2)-Zn(1)-N(1)-C(1)	-178.3(2)
O(1)-Zn(1)-N(1)-C(5)	-176.1(2)
O(3)-Zn(1)-N(1)-C(5)	-58.9(2)
N(2)-Zn(1)-N(1)-C(5)	64.5(2)
O(1)-Zn(1)-N(2)-C(12)	50.7(3)
O(3)-Zn(1)-N(2)-C(12)	-86.9(3)
N(1)-Zn(1)-N(2)-C(12)	-179.7(3)
O(1)-Zn(1)-N(2)-C(7)	167.8(2)
O(3)-Zn(1)-N(2)-C(7)	30.2(3)
N(1)-Zn(1)-N(2)-C(7)	-62.5(2)
O(1)-Zn(1)-N(2)-C(8)	-72.5(3)

O(3)-Zn(1)-N(2)-C(8)	149.9(2)
N(1)-Zn(1)-N(2)-C(8)	57.2(2)
O(7)-Zn(2)-N(3)-C(24)	-58.2(3)
O(5)-Zn(2)-N(3)-C(24)	65.6(2)
N(4)-Zn(2)-N(3)-C(24)	-177.7(2)
O(7)-Zn(2)-N(3)-C(33)	62.7(3)
O(5)-Zn(2)-N(3)-C(33)	-173.6(2)
N(4)-Zn(2)-N(3)-C(33)	-56.8(2)
O(7)-Zn(2)-N(3)-C(28)	-175.7(2)
O(5)-Zn(2)-N(3)-C(28)	-52.0(2)
N(4)-Zn(2)-N(3)-C(28)	64.8(2)
O(7)-Zn(2)-N(4)-C(35)	52.4(3)
O(5)-Zn(2)-N(4)-C(35)	-83.8(3)
N(3)-Zn(2)-N(4)-C(35)	179.9(3)
O(7)-Zn(2)-N(4)-C(31)	-70.8(3)
O(5)-Zn(2)-N(4)-C(31)	153.0(2)
N(3)-Zn(2)-N(4)-C(31)	56.7(3)
O(7)-Zn(2)-N(4)-C(30)	169.8(2)
O(5)-Zn(2)-N(4)-C(30)	33.7(3)
N(3)-Zn(2)-N(4)-C(30)	-62.6(2)
C(10)-N(1)-C(1)-C(2)	74.9(4)
C(5)-N(1)-C(1)-C(2)	-52.2(4)
Zn(1)-N(1)-C(1)-C(2)	-165.7(3)
N(1)-C(1)-C(2)-C(3)	57.0(5)
C(1)-C(2)-C(3)-C(4)	-58.0(5)
C(2)-C(3)-C(4)-C(5)	57.2(5)
C(10)-N(1)-C(5)-C(6)	48.6(4)
C(1)-N(1)-C(5)-C(6)	174.6(3)
Zn(1)-N(1)-C(5)-C(6)	-72.0(3)
C(10)-N(1)-C(5)-C(4)	-76.8(4)
C(1)-N(1)-C(5)-C(4)	49.2(4)
Zn(1)-N(1)-C(5)-C(4)	162.6(3)
C(3)-C(4)-C(5)-N(1)	-53.4(4)
C(3)-C(4)-C(5)-C(6)	-179.1(3)
N(1)-C(5)-C(6)-C(11)	-55.6(4)
C(4)-C(5)-C(6)-C(11)	70.9(4)
N(1)-C(5)-C(6)-C(7)	67.2(4)
C(4)-C(5)-C(6)-C(7)	-166.3(3)
C(12)-N(2)-C(7)-C(6)	-170.4(3)
C(8)-N(2)-C(7)-C(6)	-51.7(4)
Zn(1)-N(2)-C(7)-C(6)	69.4(3)
C(5)-C(6)-C(7)-N(2)	-66.4(4)
C(11)-C(6)-C(7)-N(2)	58.0(4)
C(12)-N(2)-C(8)-C(15)	-61.8(4)
C(7)-N(2)-C(8)-C(15)	-179.6(3)
Zn(1)-N(2)-C(8)-C(15)	63.2(3)
C(12)-N(2)-C(8)-C(9)	170.8(3)
C(7)-N(2)-C(8)-C(9)	53.0(4)
Zn(1)-N(2)-C(8)-C(9)	-64.2(3)
N(2)-C(8)-C(9)-C(11)	-61.6(4)
C(15)-C(8)-C(9)-C(11)	173.8(3)
N(2)-C(8)-C(9)-C(10)	62.6(4)
C(15)-C(8)-C(9)-C(10)	-62.0(4)
C(1)-N(1)-C(10)-C(9)	-176.2(3)
C(5)-N(1)-C(10)-C(9)	-50.4(4)
Zn(1)-N(1)-C(10)-C(9)	67.4(3)
C(11)-C(9)-C(10)-N(1)	58.2(4)

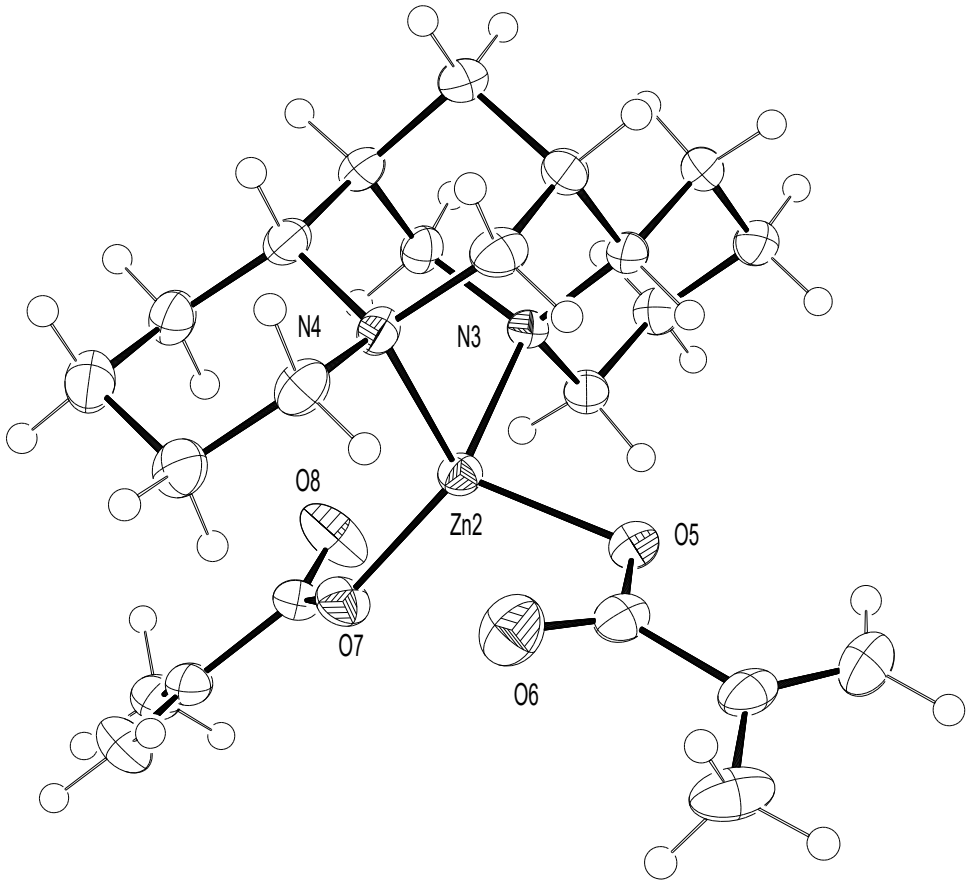
C(8)-C(9)-C(10)-N(1)	-65.3(4)
C(10)-C(9)-C(11)-C(6)	-62.9(4)
C(8)-C(9)-C(11)-C(6)	65.8(4)
C(5)-C(6)-C(11)-C(9)	62.6(4)
C(7)-C(6)-C(11)-C(9)	-63.4(4)
C(7)-N(2)-C(12)-C(13)	179.9(3)
C(8)-N(2)-C(12)-C(13)	60.7(4)
Zn(1)-N(2)-C(12)-C(13)	-64.1(4)
N(2)-C(12)-C(13)-C(14)	-55.5(5)
C(12)-C(13)-C(14)-C(15)	51.0(5)
N(2)-C(8)-C(15)-C(14)	58.9(4)
C(9)-C(8)-C(15)-C(14)	-175.1(3)
C(13)-C(14)-C(15)-C(8)	-53.6(5)
Zn(1)-O(1)-C(16)-O(2)	2.3(5)
Zn(1)-O(1)-C(16)-C(17)	-177.0(2)
O(2)-C(16)-C(17)-C(19)	20.3(6)
O(1)-C(16)-C(17)-C(19)	-160.4(4)
O(2)-C(16)-C(17)-C(18)	-158.5(4)
O(1)-C(16)-C(17)-C(18)	20.9(5)
Zn(1)-O(3)-C(20)-O(4)	-3.9(5)
Zn(1)-O(3)-C(20)-C(21)	177.6(3)
O(4)-C(20)-C(21)-C(23)	-174.9(4)
O(3)-C(20)-C(21)-C(23)	3.7(6)
O(4)-C(20)-C(21)-C(22)	5.9(6)
O(3)-C(20)-C(21)-C(22)	-175.6(4)
C(33)-N(3)-C(24)-C(25)	71.9(4)
C(28)-N(3)-C(24)-C(25)	-52.8(4)
Zn(2)-N(3)-C(24)-C(25)	-168.5(3)
N(3)-C(24)-C(25)-C(26)	55.5(4)
C(24)-C(25)-C(26)-C(27)	-55.4(4)
C(25)-C(26)-C(27)-C(28)	56.4(4)
C(24)-N(3)-C(28)-C(27)	51.1(4)
C(33)-N(3)-C(28)-C(27)	-73.2(4)
Zn(2)-N(3)-C(28)-C(27)	166.7(2)
C(24)-N(3)-C(28)-C(29)	176.0(3)
C(33)-N(3)-C(28)-C(29)	51.7(4)
Zn(2)-N(3)-C(28)-C(29)	-68.4(3)
C(26)-C(27)-C(28)-N(3)	-54.9(4)
C(26)-C(27)-C(28)-C(29)	-179.3(3)
N(3)-C(28)-C(29)-C(30)	63.6(4)
C(27)-C(28)-C(29)-C(30)	-170.7(3)
N(3)-C(28)-C(29)-C(34)	-59.6(4)
C(27)-C(28)-C(29)-C(34)	66.2(4)
C(35)-N(4)-C(30)-C(29)	-168.8(3)
C(31)-N(4)-C(30)-C(29)	-51.0(4)
Zn(2)-N(4)-C(30)-C(29)	70.3(3)
C(34)-C(29)-C(30)-N(4)	57.3(4)
C(28)-C(29)-C(30)-N(4)	-66.9(4)
C(35)-N(4)-C(31)-C(38)	-61.9(4)
C(30)-N(4)-C(31)-C(38)	179.9(3)
Zn(2)-N(4)-C(31)-C(38)	64.2(4)
C(35)-N(4)-C(31)-C(32)	170.8(3)
C(30)-N(4)-C(31)-C(32)	52.7(4)
Zn(2)-N(4)-C(31)-C(32)	-63.1(4)
N(4)-C(31)-C(32)-C(33)	62.3(4)
C(38)-C(31)-C(32)-C(33)	-63.2(4)
N(4)-C(31)-C(32)-C(34)	-62.7(4)

C(38)-C(31)-C(32)-C(34)	171.8(3)
C(24)-N(3)-C(33)-C(32)	-174.7(3)
C(28)-N(3)-C(33)-C(32)	-51.3(4)
Zn(2)-N(3)-C(33)-C(32)	67.4(4)
C(34)-C(32)-C(33)-N(3)	57.2(4)
C(31)-C(32)-C(33)-N(3)	-66.3(5)
C(30)-C(29)-C(34)-C(32)	-63.6(4)
C(28)-C(29)-C(34)-C(32)	63.5(4)
C(33)-C(32)-C(34)-C(29)	-61.7(4)
C(31)-C(32)-C(34)-C(29)	67.0(4)
C(31)-N(4)-C(35)-C(36)	61.0(4)
C(30)-N(4)-C(35)-C(36)	-179.8(3)
Zn(2)-N(4)-C(35)-C(36)	-64.9(4)
N(4)-C(35)-C(36)-C(37)	-57.0(4)
C(35)-C(36)-C(37)-C(38)	52.0(5)
N(4)-C(31)-C(38)-C(37)	59.1(4)
C(32)-C(31)-C(38)-C(37)	-175.1(3)
C(36)-C(37)-C(38)-C(31)	-53.2(5)
Zn(2)-O(5)-C(39)-O(6)	-1.8(5)
Zn(2)-O(5)-C(39)-C(40)	178.7(3)
O(6)-C(39)-C(40)-C(42)	-173.1(4)
O(5)-C(39)-C(40)-C(42)	6.4(6)
O(6)-C(39)-C(40)-C(41)	6.9(6)
O(5)-C(39)-C(40)-C(41)	-173.6(3)
Zn(2)-O(7)-C(43)-O(8)	12.2(6)
Zn(2)-O(7)-C(43)-C(44)	-165.8(2)
O(8)-C(43)-C(44)-C(46)	-166.6(4)
O(7)-C(43)-C(44)-C(46)	11.4(6)
O(8)-C(43)-C(44)-C(45)	12.5(6)
O(7)-C(43)-C(44)-C(45)	-169.4(4)

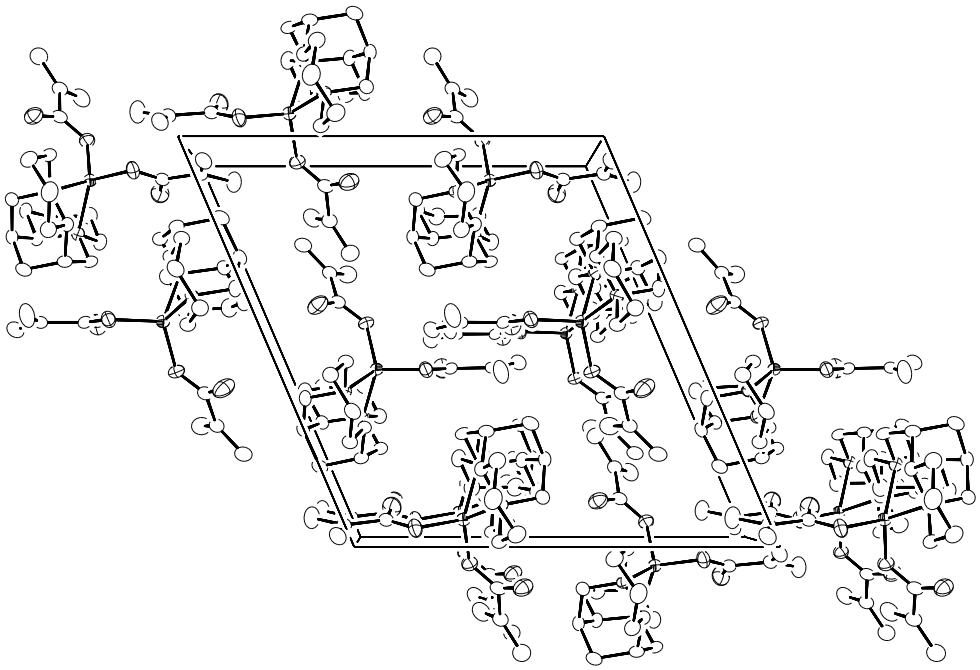
Symmetry transformations used to generate equivalent atoms:



Crystal structure of ZMS



Crystal structure of ZMS



Crystal structure of ZMS

Crystallographic details of ZAS 61

Table 1. Crystal data and structure refinement for ZAS.

Identification code	ZAS
Empirical formula	C21 H32 N2 O4 Zn
Formula weight	441.86
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 7.7634(6) A alpha = 90 deg. b = 10.9958(9) A beta = 90 deg. c = 24.578(2) A gamma = 90 deg.
Volume	2098.1(3) A^3
Z, Calculated density	4, 1.399 Mg/m^3
Absorption coefficient	1.199 mm^-1
F(000)	936
Crystal size	0.30 x 0.12 x 0.08 mm
Theta range for data collection	3.10 to 27.36 deg.
Limiting indices	-10<=h<=10, -14<=k<=14, -31<=l<=31
Reflections collected / unique	22025 / 4682 [R(int) = 0.0863]
Completeness to theta = 27.36	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.911 and 0.758
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4682 / 0 / 277
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.0748
R indices (all data)	R1 = 0.0675, wR2 = 0.0831
Absolute structure parameter	0.000(14)
Largest diff. peak and hole	0.613 and -0.418 e.A^-

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ZAS. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	6793(1)	916(1)	6419(1)	25(1)
O(1)	8320(3)	1736(2)	6949(1)	32(1)
O(2)	7637(3)	144(2)	7458(1)	42(1)
O(3)	8092(3)	-346(2)	6053(1)	35(1)
O(4)	7832(4)	482(2)	5227(1)	54(1)
N(1)	5907(4)	2527(3)	6053(1)	24(1)
N(2)	4255(4)	525(2)	6647(1)	25(1)
C(1)	7477(4)	3099(3)	5813(2)	30(1)
C(2)	7244(5)	4422(3)	5631(1)	34(1)
C(3)	6610(5)	5185(3)	6106(2)	36(1)
C(4)	4939(5)	4641(3)	6329(2)	35(1)
C(5)	5185(4)	3318(3)	6501(1)	27(1)
C(6)	3505(4)	2768(3)	6725(1)	31(1)
C(7)	2181(4)	2609(3)	6274(1)	34(1)
C(8)	2936(4)	1695(3)	5871(1)	29(1)
C(9)	4591(4)	2227(3)	5624(1)	28(1)
C(10)	3733(4)	1544(3)	7013(1)	30(1)
C(11)	3090(5)	459(3)	6156(1)	28(1)
C(12)	3651(5)	-589(3)	5793(1)	31(1)
C(13)	3622(5)	-1796(3)	6097(2)	35(1)
C(14)	4639(5)	-1720(3)	6624(2)	34(1)
C(15)	4100(5)	-635(3)	6958(1)	31(1)
C(16)	8386(4)	1129(3)	7393(1)	27(1)
C(17)	9404(5)	1653(4)	7853(2)	35(1)
C(18)	10143(5)	2740(4)	7824(2)	41(1)
C(19)	8298(6)	-342(3)	5530(2)	36(1)
C(20)	9181(5)	-1429(4)	5289(2)	42(1)
C(21)	9469(6)	-2448(4)	5540(2)	44(1)

Table 3. Bond lengths [A] and angles [deg] for ZAS.

Zn(1)-O(3)	1.938(2)
Zn(1)-O(1)	1.978(2)
Zn(1)-N(2)	2.092(3)
Zn(1)-N(1)	2.102(3)
O(1)-C(16)	1.280(4)
O(2)-C(16)	1.239(4)
O(3)-C(19)	1.294(4)
O(4)-C(19)	1.228(5)
N(1)-C(1)	1.492(4)
N(1)-C(9)	1.504(4)
N(1)-C(5)	1.512(4)
N(2)-C(15)	1.493(4)
N(2)-C(10)	1.494(4)
N(2)-C(11)	1.509(4)

C(1)-C(2)	1.533(5)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.519(5)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.530(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.527(5)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.540(5)
C(5)-H(5)	1.0000
C(6)-C(7)	1.522(5)
C(6)-C(10)	1.531(5)
C(6)-H(6)	1.0000
C(7)-C(8)	1.527(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(11)	1.534(4)
C(8)-C(9)	1.536(5)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.520(5)
C(11)-H(11)	1.0000
C(12)-C(13)	1.524(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.519(5)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.509(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.495(5)
C(17)-C(18)	1.328(6)
C(17)-H(17)	1.11(3)
C(18)-H(18B)	0.99(4)
C(18)-H(18A)	1.00(4)
C(19)-C(20)	1.500(5)
C(20)-C(21)	1.299(6)
C(20)-H(20)	1.00(4)
C(21)-H(21A)	0.94(4)
C(21)-H(21B)	0.97(3)

O(3)-Zn(1)-O(1)	108.67(11)
O(3)-Zn(1)-N(2)	117.82(11)
O(1)-Zn(1)-N(2)	118.85(11)
O(3)-Zn(1)-N(1)	125.06(11)
O(1)-Zn(1)-N(1)	95.42(10)
N(2)-Zn(1)-N(1)	88.84(11)

C(16)-O(1)-Zn(1)	110.3(2)
C(19)-O(3)-Zn(1)	121.5(2)
C(1)-N(1)-C(9)	111.8(3)
C(1)-N(1)-C(5)	110.3(3)
C(9)-N(1)-C(5)	112.6(2)
C(1)-N(1)-Zn(1)	104.9(2)
C(9)-N(1)-Zn(1)	109.7(2)
C(5)-N(1)-Zn(1)	107.10(19)
C(15)-N(2)-C(10)	108.0(3)
C(15)-N(2)-C(11)	108.7(3)
C(10)-N(2)-C(11)	110.8(3)
C(15)-N(2)-Zn(1)	112.9(2)
C(10)-N(2)-Zn(1)	105.2(2)
C(11)-N(2)-Zn(1)	111.2(2)
N(1)-C(1)-C(2)	114.7(3)
N(1)-C(1)-H(1A)	108.6
C(2)-C(1)-H(1A)	108.6
N(1)-C(1)-H(1B)	108.6
C(2)-C(1)-H(1B)	108.6
H(1A)-C(1)-H(1B)	107.6
C(3)-C(2)-C(1)	109.8(3)
C(3)-C(2)-H(2A)	109.7
C(1)-C(2)-H(2A)	109.7
C(3)-C(2)-H(2B)	109.7
C(1)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
C(2)-C(3)-C(4)	109.5(3)
C(2)-C(3)-H(3A)	109.8
C(4)-C(3)-H(3A)	109.8
C(2)-C(3)-H(3B)	109.8
C(4)-C(3)-H(3B)	109.8
H(3A)-C(3)-H(3B)	108.2
C(5)-C(4)-C(3)	111.4(3)
C(5)-C(4)-H(4A)	109.3
C(3)-C(4)-H(4A)	109.3
C(5)-C(4)-H(4B)	109.3
C(3)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	108.0
N(1)-C(5)-C(4)	113.1(3)
N(1)-C(5)-C(6)	110.4(3)
C(4)-C(5)-C(6)	111.5(3)
N(1)-C(5)-H(5)	107.1
C(4)-C(5)-H(5)	107.1
C(6)-C(5)-H(5)	107.1
C(7)-C(6)-C(10)	108.3(3)
C(7)-C(6)-C(5)	110.9(3)
C(10)-C(6)-C(5)	114.4(3)
C(7)-C(6)-H(6)	107.7
C(10)-C(6)-H(6)	107.7
C(5)-C(6)-H(6)	107.7
C(6)-C(7)-C(8)	106.8(3)
C(6)-C(7)-H(7A)	110.4
C(8)-C(7)-H(7A)	110.4
C(6)-C(7)-H(7B)	110.4
C(8)-C(7)-H(7B)	110.4
H(7A)-C(7)-H(7B)	108.6
C(7)-C(8)-C(11)	108.5(3)

C(7)-C(8)-C(9)	109.1(3)
C(11)-C(8)-C(9)	116.9(3)
C(7)-C(8)-H(8)	107.3
C(11)-C(8)-H(8)	107.3
C(9)-C(8)-H(8)	107.3
N(1)-C(9)-C(8)	112.0(3)
N(1)-C(9)-H(9A)	109.2
C(8)-C(9)-H(9A)	109.2
N(1)-C(9)-H(9B)	109.2
C(8)-C(9)-H(9B)	109.2
H(9A)-C(9)-H(9B)	107.9
N(2)-C(10)-C(6)	114.3(3)
N(2)-C(10)-H(10A)	108.7
C(6)-C(10)-H(10A)	108.7
N(2)-C(10)-H(10B)	108.7
C(6)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
N(2)-C(11)-C(12)	109.5(3)
N(2)-C(11)-C(8)	111.6(3)
C(12)-C(11)-C(8)	115.2(3)
N(2)-C(11)-H(11)	106.7
C(12)-C(11)-H(11)	106.7
C(8)-C(11)-H(11)	106.7
C(11)-C(12)-C(13)	111.6(3)
C(11)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12B)	109.3
C(13)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	108.0
C(14)-C(13)-C(12)	111.2(3)
C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13A)	109.4
C(14)-C(13)-H(13B)	109.4
C(12)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(15)-C(14)-C(13)	111.3(3)
C(15)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14B)	109.4
C(13)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
N(2)-C(15)-C(14)	111.9(3)
N(2)-C(15)-H(15A)	109.2
C(14)-C(15)-H(15A)	109.2
N(2)-C(15)-H(15B)	109.2
C(14)-C(15)-H(15B)	109.2
H(15A)-C(15)-H(15B)	107.9
O(2)-C(16)-O(1)	123.2(3)
O(2)-C(16)-C(17)	119.2(3)
O(1)-C(16)-C(17)	117.7(3)
C(18)-C(17)-C(16)	122.4(4)
C(18)-C(17)-H(17)	124.5(17)
C(16)-C(17)-H(17)	113.0(17)
C(17)-C(18)-H(18B)	119(2)
C(17)-C(18)-H(18A)	120(2)
H(18B)-C(18)-H(18A)	122(3)
O(4)-C(19)-O(3)	124.6(3)

O(4)-C(19)-C(20)	118.9(4)
O(3)-C(19)-C(20)	116.5(4)
C(21)-C(20)-C(19)	125.3(4)
C(21)-C(20)-H(20)	118(2)
C(19)-C(20)-H(20)	117(2)
C(20)-C(21)-H(21A)	123(3)
C(20)-C(21)-H(21B)	117(2)
H(21A)-C(21)-H(21B)	120(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ZAS. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	22(1)	29(1)	25(1)	2(1)	1(1)	0(1)
O(1)	27(1)	39(1)	29(1)	6(1)	-5(1)	-3(1)
O(2)	42(2)	33(2)	52(2)	5(1)	-1(1)	-7(1)
O(3)	29(1)	40(1)	35(1)	-5(1)	2(1)	4(1)
O(4)	78(2)	41(2)	43(2)	6(1)	18(2)	9(2)
N(1)	24(2)	29(2)	20(1)	2(1)	0(1)	-2(1)
N(2)	26(2)	27(2)	23(2)	2(1)	1(1)	-3(1)
C(1)	25(2)	37(2)	28(2)	3(2)	5(2)	-6(2)
C(2)	34(2)	34(2)	33(2)	6(2)	1(2)	-5(2)
C(3)	40(2)	29(2)	39(2)	3(2)	-4(2)	-5(2)
C(4)	36(2)	31(2)	38(2)	0(2)	2(2)	2(2)
C(5)	29(2)	28(2)	26(2)	-4(2)	1(2)	1(2)
C(6)	24(2)	30(2)	38(2)	-4(2)	5(2)	2(2)
C(7)	22(2)	34(2)	46(2)	4(2)	0(2)	2(2)
C(8)	24(2)	32(2)	32(2)	3(2)	-8(2)	0(2)
C(9)	32(2)	28(2)	23(2)	3(2)	-6(2)	1(2)
C(10)	26(2)	37(2)	26(2)	-5(2)	5(2)	-6(2)
C(11)	21(2)	35(2)	29(2)	0(1)	-7(2)	-2(2)
C(12)	33(2)	35(2)	23(2)	-1(2)	-7(2)	-5(2)
C(13)	42(2)	31(2)	33(2)	-1(2)	-1(2)	-5(2)
C(14)	35(2)	30(2)	37(2)	8(2)	-3(2)	-4(2)
C(15)	28(2)	34(2)	30(2)	5(2)	1(2)	-5(2)
C(16)	20(2)	34(2)	28(2)	0(1)	-1(2)	4(2)
C(17)	31(2)	47(2)	27(2)	1(2)	0(2)	3(2)
C(18)	33(2)	56(3)	32(2)	-10(2)	1(2)	-2(2)
C(19)	33(2)	33(2)	41(2)	-6(2)	7(2)	-7(2)
C(20)	40(2)	39(2)	46(3)	-10(2)	12(2)	-9(2)
C(21)	40(2)	38(3)	54(3)	-11(2)	4(2)	-5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ZAS.

	x	y	z	U(eq)
H(1A)	7845	2611	5495	36
H(1B)	8415	3066	6086	36
H(2A)	8355	4747	5498	40
H(2B)	6401	4460	5330	40
H(3A)	6403	6030	5984	43
H(3B)	7494	5202	6396	43
H(4A)	4549	5124	6645	42
H(4B)	4033	4686	6046	42
H(5)	6042	3314	6805	33
H(6)	3019	3355	6996	37
H(7A)	1958	3396	6091	41
H(7B)	1082	2300	6425	41
H(8)	2086	1600	5569	35
H(9A)	5089	1633	5366	33
H(9B)	4304	2974	5418	33
H(10A)	4615	1637	7301	36
H(10B)	2634	1325	7193	36
H(11)	1915	251	6294	34
H(12A)	4831	-432	5658	37
H(12B)	2873	-638	5475	37
H(13A)	2415	-2021	6179	42
H(13B)	4118	-2439	5863	42
H(14A)	4456	-2472	6838	41
H(14B)	5883	-1659	6539	41
H(15A)	2890	-742	7077	37
H(15B)	4828	-588	7288	37
H(17)	9400(40)	1070(30)	8219(13)	22(8)
H(18B)	10690(50)	3070(30)	8155(16)	39(11)
H(18A)	10130(40)	3200(30)	7475(15)	21(9)
H(21A)	9970(60)	-3130(40)	5370(18)	58(14)
H(21B)	9140(40)	-2490(30)	5922(15)	28(10)
H(20)	9430(50)	-1400(30)	4888(17)	49(12)

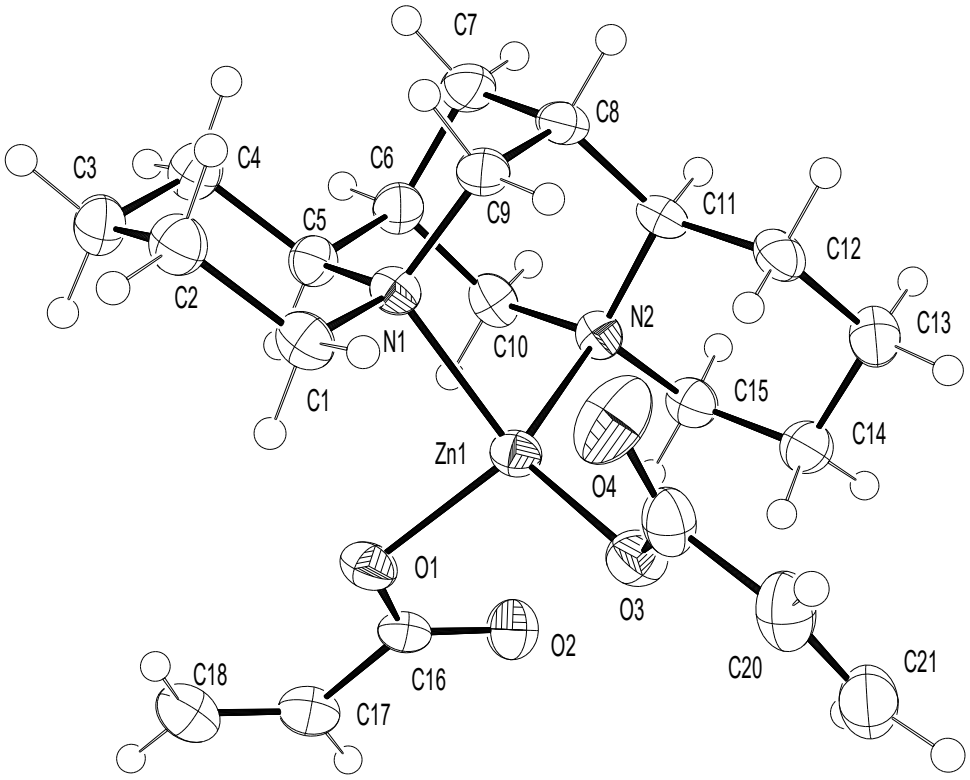
Table 6. Torsion angles [deg] for ZAS.

O(3)-Zn(1)-O(1)-C(16)	-82.9(2)
N(2)-Zn(1)-O(1)-C(16)	55.5(2)
N(1)-Zn(1)-O(1)-C(16)	147.2(2)
O(1)-Zn(1)-O(3)-C(19)	-120.5(3)
N(2)-Zn(1)-O(3)-C(19)	100.6(3)
N(1)-Zn(1)-O(3)-C(19)	-9.5(3)
O(3)-Zn(1)-N(1)-C(1)	-55.0(2)
O(1)-Zn(1)-N(1)-C(1)	62.4(2)
N(2)-Zn(1)-N(1)-C(1)	-178.8(2)
O(3)-Zn(1)-N(1)-C(9)	65.2(2)
O(1)-Zn(1)-N(1)-C(9)	-177.4(2)
N(2)-Zn(1)-N(1)-C(9)	-58.6(2)

O(3)-Zn(1)-N(1)-C(5)	-172.24(18)
O(1)-Zn(1)-N(1)-C(5)	-54.9(2)
N(2)-Zn(1)-N(1)-C(5)	64.0(2)
O(3)-Zn(1)-N(2)-C(15)	51.0(2)
O(1)-Zn(1)-N(2)-C(15)	-83.7(2)
N(1)-Zn(1)-N(2)-C(15)	-179.3(2)
O(3)-Zn(1)-N(2)-C(10)	168.53(19)
O(1)-Zn(1)-N(2)-C(10)	33.8(2)
N(1)-Zn(1)-N(2)-C(10)	-61.8(2)
O(3)-Zn(1)-N(2)-C(11)	-71.4(2)
O(1)-Zn(1)-N(2)-C(11)	153.81(18)
N(1)-Zn(1)-N(2)-C(11)	58.3(2)
C(9)-N(1)-C(1)-C(2)	74.1(4)
C(5)-N(1)-C(1)-C(2)	-52.1(4)
Zn(1)-N(1)-C(1)-C(2)	-167.1(2)
N(1)-C(1)-C(2)-C(3)	56.1(4)
C(1)-C(2)-C(3)-C(4)	-56.6(4)
C(2)-C(3)-C(4)-C(5)	57.1(4)
C(1)-N(1)-C(5)-C(4)	50.8(4)
C(9)-N(1)-C(5)-C(4)	-74.9(3)
Zn(1)-N(1)-C(5)-C(4)	164.4(2)
C(1)-N(1)-C(5)-C(6)	176.6(3)
C(9)-N(1)-C(5)-C(6)	51.0(4)
Zn(1)-N(1)-C(5)-C(6)	-69.8(3)
C(3)-C(4)-C(5)-N(1)	-54.8(4)
C(3)-C(4)-C(5)-C(6)	-180.0(3)
N(1)-C(5)-C(6)-C(7)	-57.5(4)
C(4)-C(5)-C(6)-C(7)	69.3(4)
N(1)-C(5)-C(6)-C(10)	65.3(4)
C(4)-C(5)-C(6)-C(10)	-167.9(3)
C(10)-C(6)-C(7)-C(8)	-62.9(3)
C(5)-C(6)-C(7)-C(8)	63.3(3)
C(6)-C(7)-C(8)-C(11)	65.6(3)
C(6)-C(7)-C(8)-C(9)	-62.7(3)
C(1)-N(1)-C(9)-C(8)	-177.2(3)
C(5)-N(1)-C(9)-C(8)	-52.3(4)
Zn(1)-N(1)-C(9)-C(8)	66.9(3)
C(7)-C(8)-C(9)-N(1)	58.4(4)
C(11)-C(8)-C(9)-N(1)	-65.1(4)
C(15)-N(2)-C(10)-C(6)	-169.4(3)
C(11)-N(2)-C(10)-C(6)	-50.4(4)
Zn(1)-N(2)-C(10)-C(6)	69.8(3)
C(7)-C(6)-C(10)-N(2)	57.0(4)
C(5)-C(6)-C(10)-N(2)	-67.2(4)
C(15)-N(2)-C(11)-C(12)	-61.2(3)
C(10)-N(2)-C(11)-C(12)	-179.8(3)
Zn(1)-N(2)-C(11)-C(12)	63.6(3)
C(15)-N(2)-C(11)-C(8)	170.0(3)
C(10)-N(2)-C(11)-C(8)	51.5(4)
Zn(1)-N(2)-C(11)-C(8)	-65.2(3)
C(7)-C(8)-C(11)-N(2)	-60.4(4)
C(9)-C(8)-C(11)-N(2)	63.4(4)
C(7)-C(8)-C(11)-C(12)	174.0(3)
C(9)-C(8)-C(11)-C(12)	-62.2(4)
N(2)-C(11)-C(12)-C(13)	58.1(4)
C(8)-C(11)-C(12)-C(13)	-175.1(3)
C(11)-C(12)-C(13)-C(14)	-52.6(4)

C(12)-C(13)-C(14)-C(15)	50.7(4)
C(10)-N(2)-C(15)-C(14)	-178.8(3)
C(11)-N(2)-C(15)-C(14)	61.0(4)
Zn(1)-N(2)-C(15)-C(14)	-62.9(3)
C(13)-C(14)-C(15)-N(2)	-55.9(4)
Zn(1)-O(1)-C(16)-O(2)	2.8(4)
Zn(1)-O(1)-C(16)-C(17)	-176.5(2)
O(2)-C(16)-C(17)-C(18)	-175.4(4)
O(1)-C(16)-C(17)-C(18)	3.9(5)
Zn(1)-O(3)-C(19)-O(4)	6.0(6)
Zn(1)-O(3)-C(19)-C(20)	-174.3(3)
O(4)-C(19)-C(20)-C(21)	-167.3(4)
O(3)-C(19)-C(20)-C(21)	13.0(6)

Symmetry transformations used to generate equivalent atoms:



Crystal structure of ZAS

Crystallographic details of Z3VBS 63

Table 1. Crystal data and structure refinement for Z3VBS.

Identification code	Z3VBS
Empirical formula	C33 H40 N2 O4 Zn
Formula weight	594.04
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21
Unit cell dimensions	a = 8.6170(2) A alpha = 90 deg. b = 12.0528(3) A beta = 90.446(1) deg. c = 13.7930(3) A gamma = 90 deg.
Volume	1432.48(6) A^3
Z, Calculated density	2, 1.377 Mg/m^3
Absorption coefficient	0.898 mm^-1
F(000)	628
Crystal size	0.24 x 0.20 x 0.14 mm
Theta range for data collection	3.25 to 27.53 deg.
Limiting indices	-11<=h<=11, -15<=k<=15, -17<=l<=17
Reflections collected / unique	16884 / 6407 [R(int) = 0.0318]
Completeness to theta = 27.53	99.3 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6407 / 1 / 355
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0646
R indices (all data)	R1 = 0.0334, wR2 = 0.0663
Absolute structure parameter	0.026(8)
Largest diff. peak and hole	0.513 and -0.351 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Z3VBS. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	1236(1)	1744(1)	7357(1)	24(1)
O(1)	2613(2)	1140(1)	6301(2)	52(1)
O(2)	3143(3)	189(2)	7612(1)	55(1)
O(3)	1497(2)	3341(1)	7369(1)	31(1)
O(4)	3808(2)	3260(1)	8112(1)	37(1)
N(1)	-911(2)	1254(2)	6762(1)	30(1)
N(2)	320(2)	1359(1)	8724(1)	22(1)
C(1)	-872(3)	1342(2)	5673(2)	42(1)
C(2)	-709(3)	2541(3)	5362(2)	47(1)
C(3)	-2048(3)	3241(3)	5733(2)	50(1)
C(4)	-2180(3)	3112(2)	6834(2)	41(1)
C(5)	-2273(2)	1896(2)	7129(2)	35(1)
C(6)	-2464(2)	1726(3)	8221(1)	31(1)
C(7)	-2825(3)	498(2)	8396(2)	38(1)
C(8)	-1377(3)	-147(2)	8099(2)	37(1)
C(9)	-1075(3)	59(2)	7026(2)	37(1)
C(10)	-1081(2)	2061(2)	8859(1)	25(1)
C(11)	-10(3)	143(2)	8775(2)	30(1)
C(12)	-263(3)	-279(2)	9811(2)	36(1)
C(13)	1063(3)	45(2)	10492(2)	40(1)
C(14)	1295(3)	1303(2)	10464(2)	33(1)
C(15)	1579(2)	1664(2)	9426(1)	25(1)
C(16)	3350(3)	385(2)	6744(2)	34(1)
C(17)	4468(2)	-302(2)	6170(2)	22(1)
C(18)	5145(7)	-1244(5)	6467(4)	25(2)
C(19)	6158(5)	-1848(3)	5847(4)	20(1)
C(20)	6376(5)	-1421(4)	4926(3)	22(1)
C(21)	5698(5)	-439(4)	4627(3)	26(1)
C(22)	4771(7)	148(5)	5252(4)	26(1)
C(23)	6973(5)	-2848(4)	6153(3)	29(1)
C(24)	6962(6)	-3301(6)	7030(3)	39(1)
C(25)	2700(3)	3774(2)	7791(1)	26(1)
C(26)	2618(2)	5024(2)	7875(1)	24(1)
C(27)	3597(2)	5565(2)	8533(1)	24(1)
C(28)	3504(2)	6707(2)	8684(1)	25(1)
C(29)	2423(3)	7311(2)	8140(2)	30(1)
C(30)	1464(2)	6777(3)	7478(1)	32(1)
C(31)	1549(3)	5640(2)	7352(2)	30(1)
C(32)	4520(3)	7234(2)	9412(2)	31(1)
C(33)	4798(3)	8307(2)	9513(2)	39(1)
C(21A)	6006(5)	-880(5)	4793(3)	24(1)
C(20A)	6475(5)	-1816(4)	5296(4)	21(1)
C(24A)	7595(6)	-3704(4)	6584(4)	38(1)
C(19A)	5994(5)	-2027(3)	6240(3)	21(1)
C(23A)	6522(6)	-2992(4)	6807(4)	32(1)
C(18A)	5000(7)	-1282(5)	6660(4)	22(2)
C(22A)	4985(7)	-130(5)	5234(4)	26(1)

Table 3. Bond lengths [A] and angles [deg] forZ3VBS.

Zn(1)-O(3)	1.9382(15)
Zn(1)-O(1)	2.021(2)
Zn(1)-N(2)	2.1016(16)
Zn(1)-N(1)	2.1026(18)
Zn(1)-C(16)	2.596(2)
O(1)-C(16)	1.264(3)
O(2)-C(16)	1.234(3)
O(3)-C(25)	1.294(3)
O(4)-C(25)	1.219(3)
N(1)-C(9)	1.492(3)
N(1)-C(5)	1.498(3)
N(1)-C(1)	1.506(3)
N(2)-C(10)	1.488(3)
N(2)-C(15)	1.494(2)
N(2)-C(11)	1.495(2)
C(1)-C(2)	1.515(4)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.521(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.532(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.522(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.530(3)
C(5)-H(5)	1.0000
C(6)-C(10)	1.530(3)
C(6)-C(7)	1.532(4)
C(6)-H(6)	1.0000
C(7)-C(8)	1.528(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.525(3)
C(8)-C(11)	1.537(3)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.534(3)
C(11)-H(11)	1.0000
C(12)-C(13)	1.524(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.530(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.519(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900

C(15)-H(15B)	0.9900
C(16)-C(17)	1.501(3)
C(17)-C(18)	1.339(7)
C(17)-C(22A)	1.385(6)
C(17)-C(22)	1.404(6)
C(17)-C(18A)	1.434(6)
C(18)-C(19)	1.426(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.385(6)
C(19)-C(23)	1.455(6)
C(20)-C(21)	1.382(6)
C(20)-H(20)	0.9500
C(21)-C(22)	1.375(7)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(24)	1.328(6)
C(23)-H(23)	0.9500
C(24)-H(24A)	0.9500
C(24)-H(24B)	0.9500
C(25)-C(26)	1.514(3)
C(26)-C(31)	1.382(3)
C(26)-C(27)	1.395(3)
C(27)-C(28)	1.395(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.396(3)
C(28)-C(32)	1.471(3)
C(29)-C(30)	1.385(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.383(4)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(32)-C(33)	1.322(3)
C(32)-H(32)	0.9500
C(33)-H(33A)	0.9500
C(33)-H(33B)	0.9500
C(21A)-C(20A)	1.382(7)
C(21A)-C(22A)	1.403(8)
C(21A)-H(21A)	0.9500
C(20A)-C(19A)	1.393(6)
C(20A)-H(20A)	0.9500
C(24A)-C(23A)	1.300(7)
C(24A)-H(24C)	0.9500
C(24A)-H(24D)	0.9500
C(19A)-C(18A)	1.372(7)
C(19A)-C(23A)	1.471(7)
C(23A)-H(23A)	0.9500
C(18A)-H(18A)	0.9500
C(22A)-H(22A)	0.9500

O(3)-Zn(1)-O(1)	107.21(7)
O(3)-Zn(1)-N(2)	104.82(6)
O(1)-Zn(1)-N(2)	142.47(7)
O(3)-Zn(1)-N(1)	112.61(7)
O(1)-Zn(1)-N(1)	97.89(7)
N(2)-Zn(1)-N(1)	87.29(7)
O(3)-Zn(1)-C(16)	123.23(7)
O(1)-Zn(1)-C(16)	28.45(8)

N(2)-Zn(1)-C(16)	114.94(7)
N(1)-Zn(1)-C(16)	108.25(7)
C(16)-O(1)-Zn(1)	101.93(17)
C(25)-O(3)-Zn(1)	119.77(15)
C(9)-N(1)-C(5)	109.90(18)
C(9)-N(1)-C(1)	108.33(18)
C(5)-N(1)-C(1)	108.94(18)
C(9)-N(1)-Zn(1)	105.11(15)
C(5)-N(1)-Zn(1)	114.31(13)
C(1)-N(1)-Zn(1)	110.07(13)
C(10)-N(2)-C(15)	111.36(15)
C(10)-N(2)-C(11)	113.40(16)
C(15)-N(2)-C(11)	110.39(18)
C(10)-N(2)-Zn(1)	107.31(12)
C(15)-N(2)-Zn(1)	104.54(11)
C(11)-N(2)-Zn(1)	109.39(11)
N(1)-C(1)-C(2)	110.66(19)
N(1)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	108.1
C(1)-C(2)-C(3)	111.2(2)
C(1)-C(2)-H(2A)	109.4
C(3)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2B)	109.4
C(3)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
C(2)-C(3)-C(4)	109.9(2)
C(2)-C(3)-H(3A)	109.7
C(4)-C(3)-H(3A)	109.7
C(2)-C(3)-H(3B)	109.7
C(4)-C(3)-H(3B)	109.7
H(3A)-C(3)-H(3B)	108.2
C(5)-C(4)-C(3)	111.5(2)
C(5)-C(4)-H(4A)	109.3
C(3)-C(4)-H(4A)	109.3
C(5)-C(4)-H(4B)	109.3
C(3)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	108.0
N(1)-C(5)-C(4)	111.37(18)
N(1)-C(5)-C(6)	110.8(2)
C(4)-C(5)-C(6)	113.5(2)
N(1)-C(5)-H(5)	106.9
C(4)-C(5)-H(5)	106.9
C(6)-C(5)-H(5)	106.9
C(5)-C(6)-C(10)	116.17(17)
C(5)-C(6)-C(7)	107.9(2)
C(10)-C(6)-C(7)	108.8(2)
C(5)-C(6)-H(6)	107.9
C(10)-C(6)-H(6)	107.9
C(7)-C(6)-H(6)	107.9
C(8)-C(7)-C(6)	106.40(17)
C(8)-C(7)-H(7A)	110.4
C(6)-C(7)-H(7A)	110.4
C(8)-C(7)-H(7B)	110.4
C(6)-C(7)-H(7B)	110.4

H(7A)-C(7)-H(7B)	108.6
C(9)-C(8)-C(7)	108.8(2)
C(9)-C(8)-C(11)	114.57(19)
C(7)-C(8)-C(11)	110.25(18)
C(9)-C(8)-H(8)	107.6
C(7)-C(8)-H(8)	107.6
C(11)-C(8)-H(8)	107.6
N(1)-C(9)-C(8)	114.27(17)
N(1)-C(9)-H(9A)	108.7
C(8)-C(9)-H(9A)	108.7
N(1)-C(9)-H(9B)	108.7
C(8)-C(9)-H(9B)	108.7
H(9A)-C(9)-H(9B)	107.6
N(2)-C(10)-C(6)	114.03(17)
N(2)-C(10)-H(10A)	108.7
C(6)-C(10)-H(10A)	108.7
N(2)-C(10)-H(10B)	108.7
C(6)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
N(2)-C(11)-C(12)	113.40(17)
N(2)-C(11)-C(8)	109.81(18)
C(12)-C(11)-C(8)	112.09(18)
N(2)-C(11)-H(11)	107.1
C(12)-C(11)-H(11)	107.1
C(8)-C(11)-H(11)	107.1
C(13)-C(12)-C(11)	112.21(18)
C(13)-C(12)-H(12A)	109.2
C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12B)	109.2
C(11)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
C(12)-C(13)-C(14)	109.6(2)
C(12)-C(13)-H(13A)	109.7
C(14)-C(13)-H(13A)	109.7
C(12)-C(13)-H(13B)	109.7
C(14)-C(13)-H(13B)	109.7
H(13A)-C(13)-H(13B)	108.2
C(15)-C(14)-C(13)	109.23(19)
C(15)-C(14)-H(14A)	109.8
C(13)-C(14)-H(14A)	109.8
C(15)-C(14)-H(14B)	109.8
C(13)-C(14)-H(14B)	109.8
H(14A)-C(14)-H(14B)	108.3
N(2)-C(15)-C(14)	114.76(17)
N(2)-C(15)-H(15A)	108.6
C(14)-C(15)-H(15A)	108.6
N(2)-C(15)-H(15B)	108.6
C(14)-C(15)-H(15B)	108.6
H(15A)-C(15)-H(15B)	107.6
O(2)-C(16)-O(1)	122.1(2)
O(2)-C(16)-C(17)	120.3(2)
O(1)-C(16)-C(17)	117.6(2)
O(2)-C(16)-Zn(1)	72.45(15)
O(1)-C(16)-Zn(1)	49.62(12)
C(17)-C(16)-Zn(1)	167.08(18)
C(18)-C(17)-C(22A)	105.6(4)
C(18)-C(17)-C(22)	121.3(4)

C(22A)-C(17)-C(22)	15.8(3)
C(18)-C(17)-C(18A)	11.7(4)
C(22A)-C(17)-C(18A)	117.3(4)
C(22)-C(17)-C(18A)	133.0(4)
C(18)-C(17)-C(16)	125.9(3)
C(22A)-C(17)-C(16)	128.5(3)
C(22)-C(17)-C(16)	112.8(3)
C(18A)-C(17)-C(16)	114.2(3)
C(17)-C(18)-C(19)	121.1(5)
C(17)-C(18)-H(18)	119.4
C(19)-C(18)-H(18)	119.4
C(20)-C(19)-C(18)	116.6(4)
C(20)-C(19)-C(23)	120.3(5)
C(18)-C(19)-C(23)	123.0(5)
C(21)-C(20)-C(19)	122.2(4)
C(21)-C(20)-H(20)	118.9
C(19)-C(20)-H(20)	118.9
C(22)-C(21)-C(20)	120.0(5)
C(22)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0
C(21)-C(22)-C(17)	118.7(5)
C(21)-C(22)-H(22)	120.7
C(17)-C(22)-H(22)	120.7
C(24)-C(23)-C(19)	126.7(5)
C(24)-C(23)-H(23)	116.6
C(19)-C(23)-H(23)	116.6
C(23)-C(24)-H(24A)	120.0
C(23)-C(24)-H(24B)	120.0
H(24A)-C(24)-H(24B)	120.0
O(4)-C(25)-O(3)	125.6(2)
O(4)-C(25)-C(26)	121.0(2)
O(3)-C(25)-C(26)	113.4(2)
C(31)-C(26)-C(27)	119.07(19)
C(31)-C(26)-C(25)	121.73(19)
C(27)-C(26)-C(25)	119.13(19)
C(28)-C(27)-C(26)	121.52(19)
C(28)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2
C(27)-C(28)-C(29)	118.23(19)
C(27)-C(28)-C(32)	119.6(2)
C(29)-C(28)-C(32)	122.2(2)
C(30)-C(29)-C(28)	120.3(2)
C(30)-C(29)-H(29)	119.9
C(28)-C(29)-H(29)	119.9
C(31)-C(30)-C(29)	120.7(2)
C(31)-C(30)-H(30)	119.6
C(29)-C(30)-H(30)	119.6
C(26)-C(31)-C(30)	120.2(2)
C(26)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(33)-C(32)-C(28)	126.9(2)
C(33)-C(32)-H(32)	116.6
C(28)-C(32)-H(32)	116.6
C(32)-C(33)-H(33A)	120.0
C(32)-C(33)-H(33B)	120.0
H(33A)-C(33)-H(33B)	120.0
C(20A)-C(21A)-C(22A)	119.3(4)

C(20A)-C(21A)-H(21A)	120.3
C(22A)-C(21A)-H(21A)	120.3
C(21A)-C(20A)-C(19A)	122.0(4)
C(21A)-C(20A)-H(20A)	119.0
C(19A)-C(20A)-H(20A)	119.0
C(23A)-C(24A)-H(24C)	120.0
C(23A)-C(24A)-H(24D)	120.0
H(24C)-C(24A)-H(24D)	120.0
C(18A)-C(19A)-C(20A)	117.8(4)
C(18A)-C(19A)-C(23A)	119.0(4)
C(20A)-C(19A)-C(23A)	123.3(4)
C(24A)-C(23A)-C(19A)	127.9(5)
C(24A)-C(23A)-H(23A)	116.1
C(19A)-C(23A)-H(23A)	116.1
C(19A)-C(18A)-C(17)	122.6(5)
C(19A)-C(18A)-H(18A)	118.7
C(17)-C(18A)-H(18A)	118.7
C(17)-C(22A)-C(21A)	121.0(5)
C(17)-C(22A)-H(22A)	119.5
C(21A)-C(22A)-H(22A)	119.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for Z3VBS. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	23(1)	26(1)	25(1)	-2(1)	4(1)	-7(1)
O(1)	30(1)	28(1)	99(2)	-13(1)	-7(1)	8(1)
O(2)	65(1)	52(1)	51(1)	-26(1)	41(1)	-25(1)
O(3)	32(1)	28(1)	33(1)	-2(1)	1(1)	-12(1)
O(4)	41(1)	26(1)	46(1)	3(1)	-4(1)	-2(1)
N(1)	24(1)	39(1)	28(1)	-9(1)	5(1)	-8(1)
N(2)	24(1)	17(1)	25(1)	-2(1)	4(1)	-3(1)
C(1)	29(1)	71(2)	28(1)	-13(1)	-1(1)	-11(1)
C(2)	35(1)	80(2)	26(1)	7(1)	0(1)	-6(2)
C(3)	34(1)	76(2)	42(1)	13(1)	-5(1)	-2(1)
C(4)	30(1)	54(2)	38(1)	4(1)	3(1)	2(1)
C(5)	21(1)	50(2)	33(1)	-8(1)	1(1)	-7(1)
C(6)	20(1)	39(1)	35(1)	-6(1)	7(1)	0(1)
C(7)	30(1)	42(1)	42(1)	-7(1)	11(1)	-18(1)
C(8)	38(1)	27(1)	47(1)	-9(1)	13(1)	-14(1)
C(9)	35(1)	36(1)	41(1)	-18(1)	11(1)	-18(1)
C(10)	26(1)	21(1)	27(1)	-5(1)	6(1)	0(1)
C(11)	34(1)	18(1)	37(1)	-3(1)	14(1)	-3(1)
C(12)	41(1)	22(1)	46(1)	6(1)	15(1)	-1(1)
C(13)	47(2)	35(1)	37(1)	12(1)	14(1)	8(1)
C(14)	36(1)	34(1)	28(1)	2(1)	5(1)	3(1)
C(15)	26(1)	24(1)	25(1)	0(1)	1(1)	-2(1)
C(16)	22(1)	23(1)	58(2)	-13(1)	9(1)	-8(1)
C(17)	18(1)	23(1)	27(1)	-4(1)	3(1)	-4(1)

C(25)	30(1)	25(1)	24(1)	0(1)	5(1)	-7(1)
C(26)	24(1)	25(1)	24(1)	3(1)	3(1)	-6(1)
C(27)	24(1)	25(1)	24(1)	5(1)	2(1)	-3(1)
C(28)	27(1)	24(1)	24(1)	1(1)	6(1)	-11(1)
C(29)	36(1)	23(1)	31(1)	2(1)	4(1)	-2(1)
C(30)	32(1)	33(1)	32(1)	5(1)	-3(1)	3(1)
C(31)	33(1)	30(1)	26(1)	-1(1)	-1(1)	-5(1)
C(32)	30(1)	31(1)	30(1)	-1(1)	2(1)	-7(1)
C(33)	44(1)	37(1)	36(1)	-8(1)	1(1)	-10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Z3VBS.

	x	y	z	U(eq)
H(1A)	-1840	1028	5395	51
H(1B)	12	906	5422	51
H(2A)	-683	2581	4645	56
H(2B)	282	2843	5615	56
H(3A)	-3028	3002	5417	61
H(3B)	-1871	4030	5569	61
H(4A)	-1267	3458	7152	49
H(4B)	-3120	3504	7060	49
H(5)	-3219	1581	6808	42
H(6)	-3383	2168	8433	38
H(7A)	-3059	366	9088	46
H(7B)	-3731	264	8000	46
H(8)	-1605	-955	8181	45
H(9A)	-114	-336	6842	44
H(9B)	-1941	-263	6643	44
H(10A)	-808	2842	8716	30
H(10B)	-1395	2022	9547	30
H(11)	924	-250	8519	35
H(12A)	-1246	31	10061	44
H(12B)	-362	-1097	9800	44
H(13A)	2029	-332	10291	48
H(13B)	820	-193	11161	48
H(14A)	361	1680	10718	39
H(14B)	2193	1511	10878	39
H(15A)	1712	2480	9415	30
H(15B)	2563	1329	9204	30
H(18)	4946	-1515	7101	30
H(20)	7011	-1817	4485	26
H(21)	5872	-168	3990	32
H(22)	4344	843	5066	31
H(23)	7575	-3214	5675	35
H(24A)	6378	-2968	7534	47
H(24B)	7537	-3959	7154	47
H(27)	4343	5145	8886	29
H(29)	2345	8091	8224	36
H(30)	739	7196	7106	39

H(31)	871	5282	6905	36
H(32)	5030	6753	9857	37
H(33A)	4318	8825	9087	47
H(33B)	5478	8560	10011	47
H(21A)	6372	-746	4156	29
H(20A)	7145	-2330	4988	25
H(24C)	8140	-3632	5991	45
H(24D)	7833	-4297	7014	45
H(23A)	6019	-3108	7409	38
H(18A)	4650	-1421	7300	26
H(22A)	4642	505	4885	31

Table 6. Torsion angles [deg] for Z3VBS.

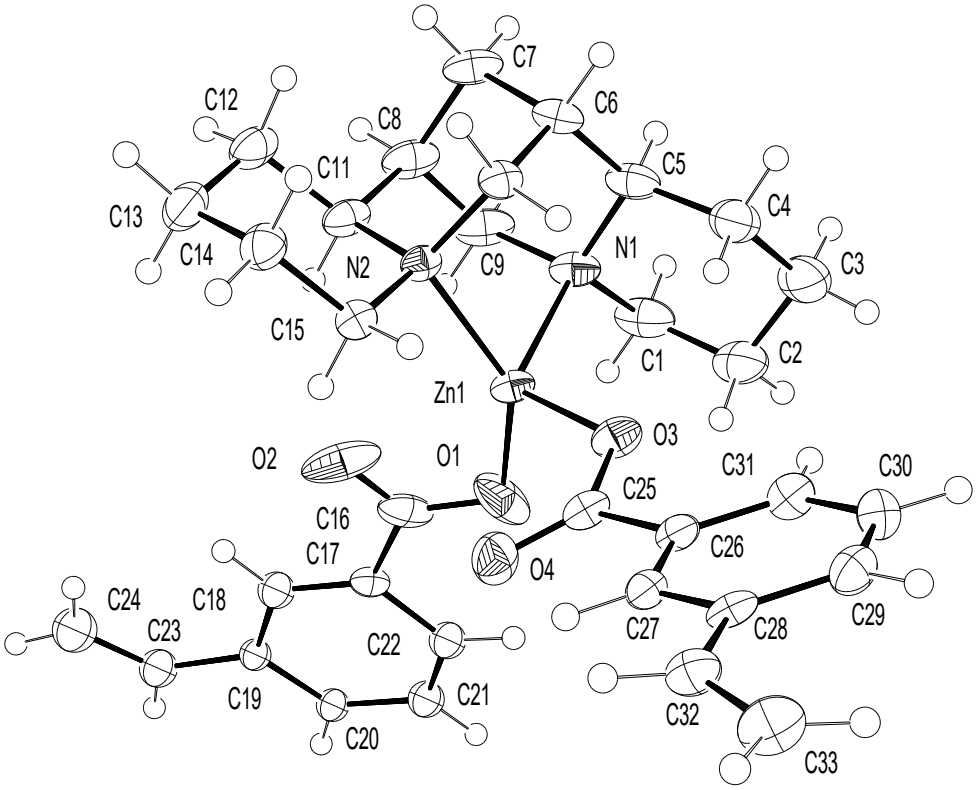
O(3)-Zn(1)-O(1)-C(16)	129.24(14)
N(2)-Zn(1)-O(1)-C(16)	-18.2(2)
N(1)-Zn(1)-O(1)-C(16)	-114.06(14)
O(1)-Zn(1)-O(3)-C(25)	-79.47(15)
N(2)-Zn(1)-O(3)-C(25)	80.70(15)
N(1)-Zn(1)-O(3)-C(25)	173.98(13)
C(16)-Zn(1)-O(3)-C(25)	-53.30(17)
O(3)-Zn(1)-N(1)-C(9)	-166.64(12)
O(1)-Zn(1)-N(1)-C(9)	80.95(13)
N(2)-Zn(1)-N(1)-C(9)	-61.71(13)
C(16)-Zn(1)-N(1)-C(9)	53.69(14)
O(3)-Zn(1)-N(1)-C(5)	-46.06(16)
O(1)-Zn(1)-N(1)-C(5)	-158.47(15)
N(2)-Zn(1)-N(1)-C(5)	58.87(15)
C(16)-Zn(1)-N(1)-C(5)	174.27(15)
O(3)-Zn(1)-N(1)-C(1)	76.92(16)
O(1)-Zn(1)-N(1)-C(1)	-35.50(17)
N(2)-Zn(1)-N(1)-C(1)	-178.15(16)
C(16)-Zn(1)-N(1)-C(1)	-62.76(17)
O(3)-Zn(1)-N(2)-C(10)	53.57(13)
O(1)-Zn(1)-N(2)-C(10)	-158.56(12)
N(1)-Zn(1)-N(2)-C(10)	-59.12(12)
C(16)-Zn(1)-N(2)-C(10)	-168.00(11)
O(3)-Zn(1)-N(2)-C(15)	-64.80(14)
O(1)-Zn(1)-N(2)-C(15)	83.08(17)
N(1)-Zn(1)-N(2)-C(15)	-177.48(14)
C(16)-Zn(1)-N(2)-C(15)	73.63(14)
O(3)-Zn(1)-N(2)-C(11)	176.98(14)
O(1)-Zn(1)-N(2)-C(11)	-35.14(19)
N(1)-Zn(1)-N(2)-C(11)	64.30(14)
C(16)-Zn(1)-N(2)-C(11)	-44.59(15)
C(9)-N(1)-C(1)-C(2)	179.9(2)
C(5)-N(1)-C(1)-C(2)	60.4(3)
Zn(1)-N(1)-C(1)-C(2)	-65.7(2)
N(1)-C(1)-C(2)-C(3)	-59.2(3)
C(1)-C(2)-C(3)-C(4)	54.5(3)
C(2)-C(3)-C(4)-C(5)	-53.0(3)
C(9)-N(1)-C(5)-C(4)	-177.50(19)

C(1)-N(1)-C(5)-C(4)	-59.0(2)
Zn(1)-N(1)-C(5)-C(4)	64.6(2)
C(9)-N(1)-C(5)-C(6)	55.2(3)
C(1)-N(1)-C(5)-C(6)	173.8(2)
Zn(1)-N(1)-C(5)-C(6)	-62.7(2)
C(3)-C(4)-C(5)-N(1)	56.2(3)
C(3)-C(4)-C(5)-C(6)	-177.96(18)
N(1)-C(5)-C(6)-C(10)	58.8(3)
C(4)-C(5)-C(6)-C(10)	-67.3(3)
N(1)-C(5)-C(6)-C(7)	-63.6(2)
C(4)-C(5)-C(6)-C(7)	170.25(19)
C(5)-C(6)-C(7)-C(8)	65.6(2)
C(10)-C(6)-C(7)-C(8)	-61.2(2)
C(6)-C(7)-C(8)-C(9)	-61.2(2)
C(6)-C(7)-C(8)-C(11)	65.2(2)
C(5)-N(1)-C(9)-C(8)	-52.3(3)
C(1)-N(1)-C(9)-C(8)	-171.2(2)
Zn(1)-N(1)-C(9)-C(8)	71.2(2)
C(7)-C(8)-C(9)-N(1)	56.3(3)
C(11)-C(8)-C(9)-N(1)	-67.7(3)
C(15)-N(2)-C(10)-C(6)	-175.05(17)
C(11)-N(2)-C(10)-C(6)	-49.8(2)
Zn(1)-N(2)-C(10)-C(6)	71.10(18)
C(5)-C(6)-C(10)-N(2)	-67.0(3)
C(7)-C(6)-C(10)-N(2)	55.0(2)
C(10)-N(2)-C(11)-C(12)	-75.7(2)
C(15)-N(2)-C(11)-C(12)	50.0(2)
Zn(1)-N(2)-C(11)-C(12)	164.54(15)
C(10)-N(2)-C(11)-C(8)	50.5(2)
C(15)-N(2)-C(11)-C(8)	176.29(15)
Zn(1)-N(2)-C(11)-C(8)	-69.20(17)
C(9)-C(8)-C(11)-N(2)	63.6(2)
C(7)-C(8)-C(11)-N(2)	-59.6(2)
C(9)-C(8)-C(11)-C(12)	-169.37(19)
C(7)-C(8)-C(11)-C(12)	67.4(2)
N(2)-C(11)-C(12)-C(13)	-52.8(3)
C(8)-C(11)-C(12)-C(13)	-177.83(18)
C(11)-C(12)-C(13)-C(14)	55.2(2)
C(12)-C(13)-C(14)-C(15)	-56.3(2)
C(10)-N(2)-C(15)-C(14)	73.2(2)
C(11)-N(2)-C(15)-C(14)	-53.7(2)
Zn(1)-N(2)-C(15)-C(14)	-171.25(16)
C(13)-C(14)-C(15)-N(2)	57.5(3)
Zn(1)-O(1)-C(16)-O(2)	-0.7(3)
Zn(1)-O(1)-C(16)-C(17)	177.43(15)
O(3)-Zn(1)-C(16)-O(2)	117.17(14)
O(1)-Zn(1)-C(16)-O(2)	179.4(2)
N(2)-Zn(1)-C(16)-O(2)	-12.76(16)
N(1)-Zn(1)-C(16)-O(2)	-108.41(14)
O(3)-Zn(1)-C(16)-O(1)	-62.18(16)
N(2)-Zn(1)-C(16)-O(1)	167.89(14)
N(1)-Zn(1)-C(16)-O(1)	72.24(15)
O(3)-Zn(1)-C(16)-C(17)	-72.4(7)
O(1)-Zn(1)-C(16)-C(17)	-10.2(6)
N(2)-Zn(1)-C(16)-C(17)	157.6(6)
N(1)-Zn(1)-C(16)-C(17)	62.0(7)
O(2)-C(16)-C(17)-C(18)	10.3(5)

O(1)-C(16)-C(17)-C(18)	-167.9(4)
Zn(1)-C(16)-C(17)-C(18)	-159.1(6)
O(2)-C(16)-C(17)-C(22A)	-171.8(3)
O(1)-C(16)-C(17)-C(22A)	10.1(4)
Zn(1)-C(16)-C(17)-C(22A)	18.9(8)
O(2)-C(16)-C(17)-C(22)	-169.4(3)
O(1)-C(16)-C(17)-C(22)	12.4(4)
Zn(1)-C(16)-C(17)-C(22)	21.2(8)
O(2)-C(16)-C(17)-C(18A)	11.1(4)
O(1)-C(16)-C(17)-C(18A)	-167.1(3)
Zn(1)-C(16)-C(17)-C(18A)	-158.3(6)
C(22A)-C(17)-C(18)-C(19)	-0.2(6)
C(22)-C(17)-C(18)-C(19)	-2.2(7)
C(18A)-C(17)-C(18)-C(19)	174(3)
C(16)-C(17)-C(18)-C(19)	178.1(4)
C(17)-C(18)-C(19)-C(20)	-1.2(7)
C(17)-C(18)-C(19)-C(23)	177.1(4)
C(18)-C(19)-C(20)-C(21)	2.4(6)
C(23)-C(19)-C(20)-C(21)	-176.0(4)
C(19)-C(20)-C(21)-C(22)	-0.1(7)
C(20)-C(21)-C(22)-C(17)	-3.3(7)
C(18)-C(17)-C(22)-C(21)	4.5(7)
C(22A)-C(17)-C(22)-C(21)	-2.5(12)
C(18A)-C(17)-C(22)-C(21)	3.6(7)
C(16)-C(17)-C(22)-C(21)	-175.8(4)
C(20)-C(19)-C(23)-C(24)	174.8(5)
C(18)-C(19)-C(23)-C(24)	-3.5(7)
Zn(1)-O(3)-C(25)-O(4)	7.8(3)
Zn(1)-O(3)-C(25)-C(26)	-171.10(12)
O(4)-C(25)-C(26)-C(31)	166.6(2)
O(3)-C(25)-C(26)-C(31)	-14.4(3)
O(4)-C(25)-C(26)-C(27)	-16.5(3)
O(3)-C(25)-C(26)-C(27)	162.50(17)
C(31)-C(26)-C(27)-C(28)	1.0(3)
C(25)-C(26)-C(27)-C(28)	-176.01(17)
C(26)-C(27)-C(28)-C(29)	-1.5(3)
C(26)-C(27)-C(28)-C(32)	177.66(17)
C(27)-C(28)-C(29)-C(30)	0.7(3)
C(32)-C(28)-C(29)-C(30)	-178.45(18)
C(28)-C(29)-C(30)-C(31)	0.7(3)
C(27)-C(26)-C(31)-C(30)	0.4(3)
C(25)-C(26)-C(31)-C(30)	177.29(18)
C(29)-C(30)-C(31)-C(26)	-1.2(3)
C(27)-C(28)-C(32)-C(33)	165.8(2)
C(29)-C(28)-C(32)-C(33)	-15.1(3)
C(22A)-C(21A)-C(20A)-C(19A)	-1.6(6)
C(21A)-C(20A)-C(19A)-C(18A)	1.3(6)
C(21A)-C(20A)-C(19A)-C(23A)	-177.4(4)
C(18A)-C(19A)-C(23A)-C(24A)	-170.8(5)
C(20A)-C(19A)-C(23A)-C(24A)	7.9(7)
C(20A)-C(19A)-C(18A)-C(17)	-0.9(7)
C(23A)-C(19A)-C(18A)-C(17)	177.9(4)
C(18)-C(17)-C(18A)-C(19A)	-5.1(19)
C(22A)-C(17)-C(18A)-C(19A)	0.8(7)
C(22)-C(17)-C(18A)-C(19A)	-1.1(8)
C(16)-C(17)-C(18A)-C(19A)	178.2(4)
C(18)-C(17)-C(22A)-C(21A)	0.2(6)

C(22)-C(17)-C(22A)-C(21A)	174.0(18)
C(18A)-C(17)-C(22A)-C(21A)	-1.0(6)
C(16)-C(17)-C(22A)-C(21A)	-178.1(3)
C(20A)-C(21A)-C(22A)-C(17)	1.4(7)

Symmetry transformations used to generate equivalent atoms:



Showing atom labels. Disordered component omitted.

Crystal structure of Z3VBS

Crystallographic details of ZADAC 67

Table 1. Crystal data and structure refinement for ZADAC.

Identification code	ZADAC
Empirical formula	C13 H24 N2 O5 Zn
Formula weight	353.71
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2
Unit cell dimensions	a = 18.5904(6) A alpha = 90 deg. b = 8.5393(3) A beta = 106.848(2) deg. c = 22.3795(6) A gamma = 90 deg.
Volume	3400.23(19) A^3
Z, Calculated density	8, 1.382 Mg/m^3
Absorption coefficient	1.465 mm^-1
F(000)	1488
Crystal size	0.24 x 0.12 x 0.03 mm
Theta range for data collection	2.92 to 29.15 deg.
Limiting indices	-24<=h<=24, -11<=k<=11, -28<=l<=29
Reflections collected / unique	22356 / 7574 [R(int) = 0.0586]
Completeness to theta = 26.00	97.1 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7574 / 1 / 381
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.0844
R indices (all data)	R1 = 0.0790, wR2 = 0.0975
Absolute structure parameter	0.040(17)
Largest diff. peak and hole	0.455 and -0.643 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ZADAC. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	6812(1)	5166(1)	5425(1)	27(1)
Zn(2)	8161(1)	7529(1)	9544(1)	26(1)
O(1)	7663(2)	3820(5)	5847(2)	38(1)
O(2)	7880(2)	5426(7)	6651(2)	63(1)
O(3)	6439(2)	3928(5)	4662(2)	32(1)
O(4)	5492(2)	5623(5)	4480(2)	39(1)
O(5)	7298(2)	8807(5)	9087(2)	35(1)
O(6)	7017(2)	6858(6)	8403(2)	49(1)
O(7)	8485(2)	8841(4)	10291(1)	30(1)
O(8)	9497(2)	7343(5)	10597(2)	40(1)
O(1S)	8460(2)	7092(5)	7714(2)	53(1)
O(2S)	6430(2)	5184(6)	7319(2)	49(1)
N(1)	7045(2)	7436(7)	5272(2)	30(1)
N(2)	6177(2)	5977(5)	5957(2)	24(1)
N(3)	8883(2)	6690(6)	9098(2)	28(1)
N(4)	7947(2)	5260(6)	9728(2)	27(1)
C(1)	6482(2)	8380(6)	5460(2)	29(1)
C(2)	6681(3)	10105(10)	5543(3)	40(1)
C(3)	6126(3)	11037(8)	5789(3)	51(2)
C(4)	6016(3)	10304(6)	6376(2)	49(1)
C(5)	5789(3)	8604(7)	6263(3)	43(2)
C(6)	6372(2)	7672(5)	6051(2)	29(1)
C(7)	8025(3)	4240(9)	6399(3)	42(2)
C(10)	5808(3)	4480(8)	4326(2)	33(1)
C(11)	5438(3)	3726(8)	3704(2)	49(2)
C(12)	5703(3)	2534(9)	3506(3)	68(2)
C(13)	8998(2)	5031(5)	9278(2)	30(1)
C(14)	9331(3)	4105(7)	8841(3)	46(2)
C(15)	9431(3)	2385(6)	9026(3)	56(1)
C(16)	8686(3)	1669(8)	9043(3)	53(2)
C(17)	8351(3)	2589(9)	9484(2)	40(1)
C(18)	8256(2)	4310(6)	9302(2)	30(1)
C(19)	6895(3)	8184(9)	8585(3)	40(2)
C(20)	6231(3)	9134(11)	8233(3)	72(2)
C(22)	9094(3)	8396(7)	10692(2)	27(1)
C(1S)	8139(4)	8607(10)	7558(3)	66(2)
C(23)	9265(3)	9253(7)	11298(2)	39(1)
C(24)	9829(3)	8852(7)	11789(2)	52(1)
C(2S)	6825(4)	3769(9)	7480(3)	65(2)
C(8)	8608(7)	3421(17)	6840(7)	57(4)
C(9)	8773(9)	2047(19)	6702(7)	70(4)
C(21)	6052(6)	10329(14)	8273(5)	40(2)
C(8A)	8698(9)	2950(20)	6626(7)	69(4)
C(9A)	9150(8)	3139(19)	7186(6)	82(4)
C(21A)	5667(6)	8765(15)	7849(5)	59(3)

Table 3. Bond lengths [A] and angles [deg] for ZADAC.

Zn(1)-O(3)	1.956(3)
Zn(1)-O(1)	1.962(3)
Zn(1)-N(2)	2.025(4)
Zn(1)-N(1)	2.036(6)
Zn(2)-O(7)	1.956(3)
Zn(2)-O(5)	1.965(3)
Zn(2)-N(3)	2.023(4)
Zn(2)-N(4)	2.044(5)
O(1)-C(7)	1.275(6)
O(2)-C(7)	1.226(8)
O(3)-C(10)	1.285(6)
O(4)-C(10)	1.238(6)
O(5)-C(19)	1.271(6)
O(6)-C(19)	1.246(8)
O(7)-C(22)	1.282(5)
O(8)-C(22)	1.229(6)
O(1S)-C(1S)	1.424(8)
O(1S)-H(1S)	0.8400
O(2S)-C(2S)	1.406(8)
O(2S)-H(2S)	0.8400
N(1)-C(1)	1.475(6)
N(1)-H(1A)	0.9200
N(1)-H(1B)	0.9200
N(2)-C(6)	1.492(6)
N(2)-H(2A)	0.9200
N(2)-H(2B)	0.9200
N(3)-C(13)	1.471(6)
N(3)-H(3A)	0.9200
N(3)-H(3B)	0.9200
N(4)-C(18)	1.488(6)
N(4)-H(4A)	0.9200
N(4)-H(4B)	0.9200
C(1)-C(2)	1.517(9)
C(1)-C(6)	1.521(6)
C(1)-H(1)	1.0000
C(2)-C(3)	1.526(8)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.522(8)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.512(8)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.527(6)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6)	1.0000
C(7)-C(8)	1.422(15)
C(7)-C(8A)	1.632(18)
C(10)-C(11)	1.508(7)
C(11)-C(12)	1.266(8)
C(11)-H(11)	0.9500
C(12)-H(12A)	0.9500

C(12)-H(12B)	0.9500
C(13)-C(14)	1.522(6)
C(13)-C(18)	1.524(6)
C(13)-H(13)	1.0000
C(14)-C(15)	1.523(8)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.523(7)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.527(8)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.521(9)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18)	1.0000
C(19)-C(20)	1.497(8)
C(20)-C(21)	1.085(13)
C(20)-C(21A)	1.188(11)
C(22)-C(23)	1.492(7)
C(1S)-H(1S1)	0.9800
C(1S)-H(1S2)	0.9800
C(1S)-H(1S3)	0.9800
C(23)-C(24)	1.326(6)
C(23)-H(23)	0.9500
C(24)-H(24A)	0.9500
C(24)-H(24B)	0.9500
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800
C(2S)-H(2S3)	0.9800
C(8)-C(9)	1.27(2)
C(8)-H(8)	0.9500
C(9)-H(9A)	0.9500
C(9)-H(9B)	0.9500
C(21)-H(21A)	0.9500
C(21)-H(21B)	0.9500
C(8A)-C(9A)	1.30(2)
C(8A)-H(8A)	0.9500
C(9A)-H(9A1)	0.9500
C(9A)-H(9A2)	0.9500
C(21A)-H(21C)	0.9500
C(21A)-H(21D)	0.9500

O(3)-Zn(1)-O(1)	97.77(16)
O(3)-Zn(1)-N(2)	125.35(14)
O(1)-Zn(1)-N(2)	116.34(15)
O(3)-Zn(1)-N(1)	113.99(15)
O(1)-Zn(1)-N(1)	117.18(15)
N(2)-Zn(1)-N(1)	87.81(17)
O(7)-Zn(2)-O(5)	97.49(15)
O(7)-Zn(2)-N(3)	122.67(15)
O(5)-Zn(2)-N(3)	119.90(16)
O(7)-Zn(2)-N(4)	113.66(15)
O(5)-Zn(2)-N(4)	117.03(15)
N(3)-Zn(2)-N(4)	87.61(17)
C(7)-O(1)-Zn(1)	115.2(4)

C(10)-O(3)-Zn(1)	110.1(4)
C(19)-O(5)-Zn(2)	114.2(4)
C(22)-O(7)-Zn(2)	114.9(3)
C(1S)-O(1S)-H(1S)	109.5
C(2S)-O(2S)-H(2S)	109.5
C(1)-N(1)-Zn(1)	105.6(3)
C(1)-N(1)-H(1A)	110.6
Zn(1)-N(1)-H(1A)	110.6
C(1)-N(1)-H(1B)	110.6
Zn(1)-N(1)-H(1B)	110.6
H(1A)-N(1)-H(1B)	108.7
C(6)-N(2)-Zn(1)	104.8(3)
C(6)-N(2)-H(2A)	110.8
Zn(1)-N(2)-H(2A)	110.8
C(6)-N(2)-H(2B)	110.8
Zn(1)-N(2)-H(2B)	110.8
H(2A)-N(2)-H(2B)	108.9
C(13)-N(3)-Zn(2)	105.7(3)
C(13)-N(3)-H(3A)	110.6
Zn(2)-N(3)-H(3A)	110.6
C(13)-N(3)-H(3B)	110.6
Zn(2)-N(3)-H(3B)	110.6
H(3A)-N(3)-H(3B)	108.7
C(18)-N(4)-Zn(2)	104.7(3)
C(18)-N(4)-H(4A)	110.8
Zn(2)-N(4)-H(4A)	110.8
C(18)-N(4)-H(4B)	110.8
Zn(2)-N(4)-H(4B)	110.8
H(4A)-N(4)-H(4B)	108.9
N(1)-C(1)-C(2)	113.4(5)
N(1)-C(1)-C(6)	108.4(4)
C(2)-C(1)-C(6)	111.6(4)
N(1)-C(1)-H(1)	107.7
C(2)-C(1)-H(1)	107.7
C(6)-C(1)-H(1)	107.7
C(1)-C(2)-C(3)	112.7(5)
C(1)-C(2)-H(2A)	109.1
C(3)-C(2)-H(2A)	109.1
C(1)-C(2)-H(2B)	109.1
C(3)-C(2)-H(2B)	109.1
H(2A)-C(2)-H(2B)	107.8
C(4)-C(3)-C(2)	111.7(5)
C(4)-C(3)-H(3A)	109.3
C(2)-C(3)-H(3A)	109.3
C(4)-C(3)-H(3B)	109.3
C(2)-C(3)-H(3B)	109.3
H(3A)-C(3)-H(3B)	107.9
C(5)-C(4)-C(3)	110.6(5)
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(4)-C(5)-C(6)	111.3(4)
C(4)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5A)	109.4
C(4)-C(5)-H(5B)	109.4

C(6)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
N(2)-C(6)-C(1)	110.5(3)
N(2)-C(6)-C(5)	112.6(4)
C(1)-C(6)-C(5)	110.5(4)
N(2)-C(6)-H(6)	107.7
C(1)-C(6)-H(6)	107.7
C(5)-C(6)-H(6)	107.7
O(2)-C(7)-O(1)	123.6(6)
O(2)-C(7)-C(8)	108.2(8)
O(1)-C(7)-C(8)	128.1(9)
O(2)-C(7)-C(8A)	131.6(8)
O(1)-C(7)-C(8A)	104.7(8)
C(8)-C(7)-C(8A)	24.5(7)
O(4)-C(10)-O(3)	123.6(5)
O(4)-C(10)-C(11)	117.8(5)
O(3)-C(10)-C(11)	118.6(5)
C(12)-C(11)-C(10)	123.2(6)
C(12)-C(11)-H(11)	118.4
C(10)-C(11)-H(11)	118.4
C(11)-C(12)-H(12A)	120.0
C(11)-C(12)-H(12B)	120.0
H(12A)-C(12)-H(12B)	120.0
N(3)-C(13)-C(14)	112.2(4)
N(3)-C(13)-C(18)	109.8(4)
C(14)-C(13)-C(18)	110.6(4)
N(3)-C(13)-H(13)	108.0
C(14)-C(13)-H(13)	108.0
C(18)-C(13)-H(13)	108.0
C(13)-C(14)-C(15)	111.5(4)
C(13)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14B)	109.3
C(15)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
C(14)-C(15)-C(16)	110.7(5)
C(14)-C(15)-H(15A)	109.5
C(16)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
C(16)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	108.1
C(15)-C(16)-C(17)	110.7(5)
C(15)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	108.1
C(18)-C(17)-C(16)	111.2(5)
C(18)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17B)	109.4
C(16)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
N(4)-C(18)-C(17)	113.0(4)
N(4)-C(18)-C(13)	108.8(4)
C(17)-C(18)-C(13)	111.3(4)
N(4)-C(18)-H(18)	107.8

C(17)-C(18)-H(18)	107.8
C(13)-C(18)-H(18)	107.8
O(6)-C(19)-O(5)	123.6(6)
O(6)-C(19)-C(20)	121.3(6)
O(5)-C(19)-C(20)	115.0(7)
C(21)-C(20)-C(21A)	94.7(9)
C(21)-C(20)-C(19)	133.7(10)
C(21A)-C(20)-C(19)	131.1(10)
O(8)-C(22)-O(7)	123.7(5)
O(8)-C(22)-C(23)	122.5(4)
O(7)-C(22)-C(23)	113.8(5)
O(1S)-C(1S)-H(1S1)	109.5
O(1S)-C(1S)-H(1S2)	109.5
H(1S1)-C(1S)-H(1S2)	109.5
O(1S)-C(1S)-H(1S3)	109.5
H(1S1)-C(1S)-H(1S3)	109.5
H(1S2)-C(1S)-H(1S3)	109.5
C(24)-C(23)-C(22)	122.4(5)
C(24)-C(23)-H(23)	118.8
C(22)-C(23)-H(23)	118.8
C(23)-C(24)-H(24A)	120.0
C(23)-C(24)-H(24B)	120.0
H(24A)-C(24)-H(24B)	120.0
O(2S)-C(2S)-H(2S1)	109.5
O(2S)-C(2S)-H(2S2)	109.5
H(2S1)-C(2S)-H(2S2)	109.5
O(2S)-C(2S)-H(2S3)	109.5
H(2S1)-C(2S)-H(2S3)	109.5
H(2S2)-C(2S)-H(2S3)	109.5
C(9)-C(8)-C(7)	118.3(14)
C(9)-C(8)-H(8)	120.8
C(7)-C(8)-H(8)	120.8
C(8)-C(9)-H(9A)	120.0
C(8)-C(9)-H(9B)	120.0
H(9A)-C(9)-H(9B)	120.0
C(20)-C(21)-H(21A)	120.0
C(20)-C(21)-H(21B)	120.0
H(21A)-C(21)-H(21B)	120.0
C(9A)-C(8A)-C(7)	116.2(16)
C(9A)-C(8A)-H(8A)	121.9
C(7)-C(8A)-H(8A)	121.9
C(8A)-C(9A)-H(9A1)	120.0
C(8A)-C(9A)-H(9A2)	120.0
H(9A1)-C(9A)-H(9A2)	120.0
C(20)-C(21A)-H(21C)	120.0
C(20)-C(21A)-H(21D)	120.0
H(21C)-C(21A)-H(21D)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ZADAC. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	26(1)	25(1)	31(1)	-2(1)	9(1)	-1(1)
Zn(2)	23(1)	29(1)	28(1)	-2(1)	9(1)	-1(1)
O(1)	33(2)	35(2)	42(2)	-6(2)	6(2)	10(2)
O(2)	48(2)	98(4)	36(2)	-22(3)	0(2)	-4(3)
O(3)	28(2)	37(2)	31(2)	-7(2)	7(1)	2(2)
O(4)	32(2)	48(3)	34(2)	-3(2)	4(1)	7(2)
O(5)	31(2)	38(2)	32(2)	0(2)	3(1)	3(2)
O(6)	48(2)	57(3)	34(2)	-5(2)	1(2)	-11(2)
O(7)	23(2)	32(2)	31(2)	-7(2)	3(1)	5(2)
O(8)	32(2)	52(2)	34(2)	-9(2)	4(1)	18(2)
O(1S)	49(2)	72(3)	33(2)	-9(2)	5(2)	-7(2)
O(2S)	65(2)	55(2)	23(2)	-2(2)	6(2)	-2(2)
N(1)	26(2)	29(3)	34(2)	1(2)	10(2)	-1(2)
N(2)	21(2)	26(2)	27(2)	-3(2)	10(2)	0(2)
N(3)	29(2)	30(3)	24(2)	-7(2)	7(2)	-11(2)
N(4)	21(2)	32(3)	31(2)	-4(2)	13(2)	-1(2)
C(1)	28(2)	25(2)	32(2)	1(2)	6(2)	1(2)
C(2)	40(3)	30(4)	50(3)	5(3)	13(3)	-12(3)
C(3)	52(3)	25(3)	73(4)	-5(3)	15(3)	6(3)
C(4)	57(3)	31(3)	63(3)	-19(3)	23(3)	1(3)
C(5)	48(3)	37(4)	50(3)	-4(3)	26(3)	3(3)
C(6)	25(2)	30(2)	31(2)	-5(2)	6(2)	-1(2)
C(7)	31(3)	55(4)	38(3)	15(3)	6(2)	-1(3)
C(10)	30(3)	45(3)	25(2)	-1(2)	8(2)	-3(2)
C(11)	46(3)	62(4)	40(3)	-8(3)	13(2)	1(3)
C(12)	59(3)	88(5)	55(3)	-28(4)	13(3)	-10(4)
C(13)	27(2)	30(2)	35(2)	-3(2)	15(2)	-2(2)
C(14)	46(3)	43(4)	63(4)	-17(3)	39(3)	-10(3)
C(15)	61(3)	44(3)	77(4)	-18(3)	43(3)	2(3)
C(16)	66(4)	35(3)	73(4)	-10(3)	43(3)	-2(3)
C(17)	46(3)	26(3)	53(3)	-6(3)	21(3)	0(4)
C(18)	26(2)	36(3)	30(2)	-5(2)	11(2)	-5(2)
C(19)	23(2)	63(4)	34(3)	11(3)	6(2)	-7(3)
C(20)	31(3)	123(7)	48(3)	48(4)	-9(2)	12(4)
C(22)	25(2)	28(3)	30(2)	-5(2)	12(2)	-5(2)
C(1S)	66(4)	84(6)	45(3)	-12(4)	10(3)	-4(4)
C(23)	32(2)	45(3)	36(3)	-14(2)	4(2)	0(2)
C(24)	43(3)	77(4)	33(3)	-15(3)	5(2)	13(3)
C(2S)	93(5)	48(4)	56(4)	-8(3)	24(4)	0(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ZADAC.

	x	y	z	U(eq)
H(1S)	8203	6429	7465	79
H(2S)	6549	5798	7625	73
H(1A)	7523	7697	5508	35
H(1B)	7007	7595	4858	35
H(2A)	5674	5850	5755	29
H(2B)	6291	5460	6333	29
H(3A)	8683	6785	8673	33
H(3B)	9331	7226	9219	33
H(4A)	8181	5012	10138	32
H(4B)	7439	5093	9646	32
H(1)	5995	8287	5123	34
H(2A)	6691	10547	5137	48
H(2B)	7191	10215	5838	48
H(3A)	6314	12121	5882	61
H(3B)	5636	11088	5462	61
H(4A)	6489	10379	6721	59
H(4B)	5621	10885	6501	59
H(5A)	5297	8538	5939	51
H(5B)	5732	8142	6652	51
H(6)	6861	7753	6387	35
H(11)	4983	4166	3448	59
H(12A)	6157	2072	3753	82
H(12B)	5448	2102	3110	82
H(13)	9358	4979	9707	35
H(14A)	9824	4557	8851	55
H(14B)	8996	4193	8409	55
H(15A)	9802	2287	9443	67
H(15B)	9626	1807	8722	67
H(16A)	8767	568	9185	64
H(16B)	8330	1674	8618	64
H(17A)	7856	2140	9471	48
H(17B)	8684	2494	9916	48
H(18)	7896	4378	8873	36
H(1S1)	8357	9332	7903	99
H(1S2)	7594	8548	7486	99
H(1S3)	8246	8982	7179	99
H(23)	8958	10118	11333	46
H(24A)	10142	7991	11762	63
H(24B)	9921	9427	12167	63
H(2S1)	7365	3963	7564	98
H(2S2)	6659	3025	7133	98
H(2S3)	6727	3332	7853	98
H(8)	8869	3886	7228	68
H(9A)	8509	1595	6312	84
H(9B)	9161	1474	6988	84
H(21A)	5572	10671	8026	48
H(21B)	6377	11033	8554	48
H(8A)	8756	2118	6364	82
H(9A1)	9078	3987	7437	99
H(9A2)	9553	2427	7344	99
H(21C)	5274	9507	7704	71

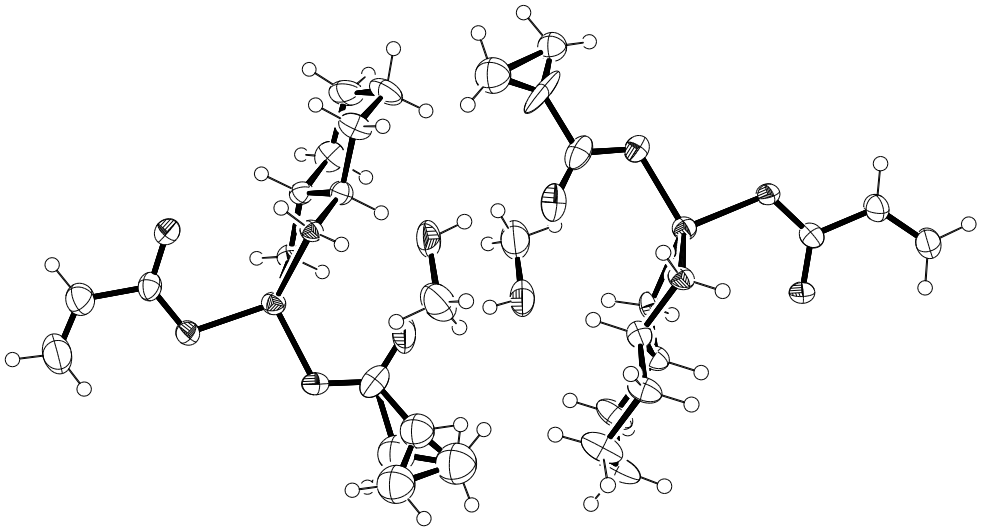
H(21D)	5610	7730	7687	71

Table 6. Torsion angles [deg] for ZADAC.

O(3)-Zn(1)-O(1)-C(7)	-175.9(4)
N(2)-Zn(1)-O(1)-C(7)	-39.9(5)
N(1)-Zn(1)-O(1)-C(7)	62.0(4)
O(1)-Zn(1)-O(3)-C(10)	172.2(3)
N(2)-Zn(1)-O(3)-C(10)	41.9(4)
N(1)-Zn(1)-O(3)-C(10)	-63.4(4)
O(7)-Zn(2)-O(5)-C(19)	-173.0(4)
N(3)-Zn(2)-O(5)-C(19)	52.3(4)
N(4)-Zn(2)-O(5)-C(19)	-51.6(4)
O(5)-Zn(2)-O(7)-C(22)	-175.4(3)
N(3)-Zn(2)-O(7)-C(22)	-42.5(4)
N(4)-Zn(2)-O(7)-C(22)	60.6(4)
O(3)-Zn(1)-N(1)-C(1)	112.3(3)
O(1)-Zn(1)-N(1)-C(1)	-134.5(3)
N(2)-Zn(1)-N(1)-C(1)	-15.8(3)
O(3)-Zn(1)-N(2)-C(6)	-130.2(3)
O(1)-Zn(1)-N(2)-C(6)	107.3(3)
N(1)-Zn(1)-N(2)-C(6)	-12.1(3)
O(7)-Zn(2)-N(3)-C(13)	103.4(3)
O(5)-Zn(2)-N(3)-C(13)	-133.5(3)
N(4)-Zn(2)-N(3)-C(13)	-13.4(3)
O(7)-Zn(2)-N(4)-C(18)	-139.8(2)
O(5)-Zn(2)-N(4)-C(18)	107.7(3)
N(3)-Zn(2)-N(4)-C(18)	-14.9(3)
Zn(1)-N(1)-C(1)-C(2)	164.8(3)
Zn(1)-N(1)-C(1)-C(6)	40.2(4)
N(1)-C(1)-C(2)-C(3)	-175.3(4)
C(6)-C(1)-C(2)-C(3)	-52.5(5)
C(1)-C(2)-C(3)-C(4)	52.2(6)
C(2)-C(3)-C(4)-C(5)	-54.4(6)
C(3)-C(4)-C(5)-C(6)	57.6(6)
Zn(1)-N(2)-C(6)-C(1)	38.0(4)
Zn(1)-N(2)-C(6)-C(5)	162.1(3)
N(1)-C(1)-C(6)-N(2)	-54.4(4)
C(2)-C(1)-C(6)-N(2)	-180.0(4)
N(1)-C(1)-C(6)-C(5)	-179.7(4)
C(2)-C(1)-C(6)-C(5)	54.7(5)
C(4)-C(5)-C(6)-N(2)	178.0(4)
C(4)-C(5)-C(6)-C(1)	-57.9(5)
Zn(1)-O(1)-C(7)-O(2)	-2.6(8)
Zn(1)-O(1)-C(7)-C(8)	172.6(8)
Zn(1)-O(1)-C(7)-C(8A)	-178.9(6)
Zn(1)-O(3)-C(10)-O(4)	-0.7(6)
Zn(1)-O(3)-C(10)-C(11)	177.8(4)
O(4)-C(10)-C(11)-C(12)	-178.6(6)
O(3)-C(10)-C(11)-C(12)	2.9(9)
Zn(2)-N(3)-C(13)-C(14)	162.7(3)
Zn(2)-N(3)-C(13)-C(18)	39.3(4)
N(3)-C(13)-C(14)-C(15)	-178.8(4)

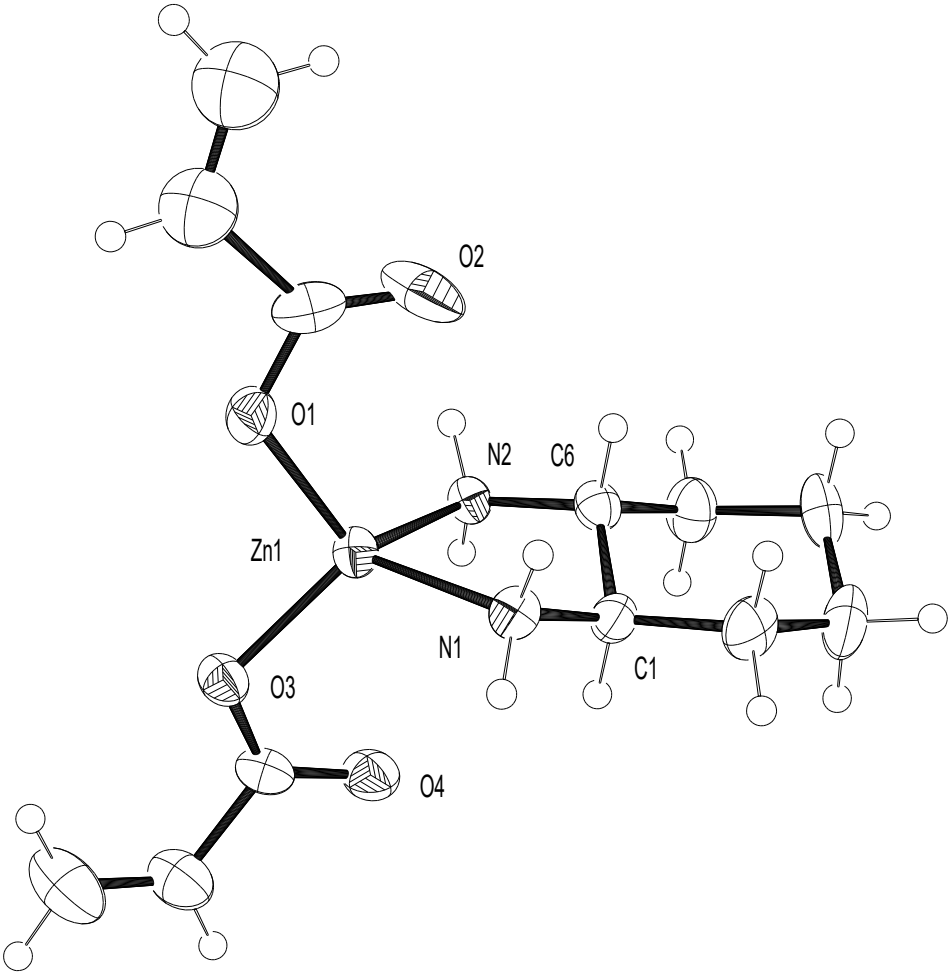
C(18)-C(13)-C(14)-C(15)	-55.9(6)
C(13)-C(14)-C(15)-C(16)	56.6(6)
C(14)-C(15)-C(16)-C(17)	-56.2(7)
C(15)-C(16)-C(17)-C(18)	56.1(7)
Zn(2)-N(4)-C(18)-C(17)	164.1(3)
Zn(2)-N(4)-C(18)-C(13)	39.9(4)
C(16)-C(17)-C(18)-N(4)	-178.7(4)
C(16)-C(17)-C(18)-C(13)	-55.8(6)
N(3)-C(13)-C(18)-N(4)	-55.1(5)
C(14)-C(13)-C(18)-N(4)	-179.4(4)
N(3)-C(13)-C(18)-C(17)	179.7(4)
C(14)-C(13)-C(18)-C(17)	55.4(5)
Zn(2)-O(5)-C(19)-O(6)	2.1(7)
Zn(2)-O(5)-C(19)-C(20)	179.5(4)
O(6)-C(19)-C(20)-C(21)	-171.9(11)
O(5)-C(19)-C(20)-C(21)	10.6(14)
O(6)-C(19)-C(20)-C(21A)	17.7(12)
O(5)-C(19)-C(20)-C(21A)	-159.8(9)
Zn(2)-O(7)-C(22)-O(8)	8.0(6)
Zn(2)-O(7)-C(22)-C(23)	-170.8(3)
O(8)-C(22)-C(23)-C(24)	-5.5(8)
O(7)-C(22)-C(23)-C(24)	173.3(5)
O(2)-C(7)-C(8)-C(9)	170.5(11)
O(1)-C(7)-C(8)-C(9)	-5.3(17)
C(8A)-C(7)-C(8)-C(9)	-25.3(19)
O(2)-C(7)-C(8A)-C(9A)	4.1(18)
O(1)-C(7)-C(8A)-C(9A)	-179.9(12)
C(8)-C(7)-C(8A)-C(9A)	-16.1(16)

Symmetry transformations used to generate equivalent atoms:



Contents of asymmetric unit. Note 2 independent molecules, MeOH solvent present & disorder in 2 vinyl groups of the 4 present.

Crystal structure of ZADAC



Crystal structure of ZADAC